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Quantum mechanics of topological solitons

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Declaration

I herewith certify that all material in this dissertation which is not my own work has been properly acknowledged.

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Abstract

Topological solitons – are of broad interest in physics. They are objects with localised energy and stability ensured by their topological properties. It is possible to create them during phase transitions which break some symmetry in a frustrated system. They are ubiquitous in condensed matter, ranging from monopole excitations in spin ices to vortices in superconductors. In such situations, their behaviour has been extensively studied.

Less well understood and yet equally interesting are the symmetry-breaking phase transitions that could produce topological defects in the early universe. Grand unified theories generically admit the creation of cosmic strings and monopoles, amongst other objects.

There is no reason to expect that the behaviour of such objects should be classical or, indeed, supersymmetric, so to fully understand the behaviour of these theories it is necessary to study the quantum properties of the associated topological defects. Unfortunately, the standard analytical tools for studying quantum field theory – including perturbation theory – do not work so well when applied to topological defects.

Motivated by this realisation, this thesis presents numerical techniques for the study of topological solitons in quantum field theory. Calculations are carried out nonperturbatively within the framework of lattice Monte Carlo simulations. Methods are demonstrated which use correlation functions to study the mass, interaction form factors, dispersion relations and excitations of quantum topological solitons. Results are compared to exact expressions obtained from integrability, and to previous work using less sophisticated numerical techniques.

The techniques developed are applied to the prototypical kink soliton and to the 't Hooft-Polyakov monopole.

L'étude approfondie de la nature est la source la plus féconde des découvertes mathématiques. Non seulement cette étude, en offrant aux recherches un but déterminé, a l'avantage d'exclure les questions vagues et les calculs sans issue : elle est encore un moyen assuré de former l'analyse elle-même, et d'en découvrir les éléments qu'il nous importe le plus de connaître, et que cette science doit toujours conserver: ces éléments fondamentaux sont ceux qui se reproduisent dans tous les effets naturels.

– Joseph Fourier, *Théorie Analytique de la Chaleur*

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1 Introduction

The novel work presented in this thesis emerges out of a synthesis of two rather different areas of theoretical physics: the study of topological solitons and numerical simulations of quantum field theory. We develop techniques that give far greater insight into the properties and excitations of topological defects than would ever be possible with perturbative quantum theory.

In order to put this progress into context, this chapter aims to give a broad overview – in historical context – of the physics under study. For example, while the 't Hooft-Polyakov monopole is a topological soliton, it is also a natural development in a line of enquiry stretching back nearly a millennium to the earliest written discussions of magnetism. The purpose of this introduction, therefore, is to put the exposition and novel results of the chapters that follow into some context.

1.1 Topological solitons

By the 1960s, physicists had begun to study the extended classical solutions found in field theory [95]. One can call them, generically, *topological defects* by analogy with defects in a crystal lattice: they are localised inhomogeneities that have a nontrivial character.

When localised in space, they were termed topological *solitons* by analogy with solitons in other partial differential equations, since they were localised solutions of the field equations that did not disperse under time evolution. In contrast, however, their stability was assured due to the topological nature of the boundary conditions.

The mid-1970s saw widespread interest in the role of topological defects in quantum field theory (see Ref. [77] for a review from the time); other applications ranged from interfacial phenomena in statistical mechanics (see Ref. [54]) to an effective model for quarks (see Ref. [5]). The cosmological consequences of such objects were also studied from about the same

time [85]. Despite recent observational work suggesting that inflation is predominant, cosmic strings may give an observable contribution to the cosmic microwave background radiation [10] or gravitational wave background [136]. Topological defects in the form of domain walls play a central role in string theory (as branes [116]) and in braneworld scenarios (see, for example, Ref. [128]).

Kinks are also studied in integrable systems where various dualities mean that study of their scattering can be relatively straightforward. The classic example is the sine-Gordon model. This possesses a rich variety of kinks, which can in turn be turned into fermions by making use of this model's remarkable duality with the massive Thirring model [26].

We will restrict ourselves in this thesis to techniques for studying topological solitons (such as kinks and 't Hooft-Polyakov monopoles) in quantum field theory. Much of what will be said is also applicable to topological defects (such as domain walls), and to statistical mechanical systems where fluctuations of interfaces are treated perturbatively.

With the exception of supersymmetric theories where solitons typically saturate the Bogomol'nyi bound [146], the consequences of quantising topological solitons are significant. Unfortunately, theoretical studies have been mainly limited to the classical limit in all but the simplest cases.

The techniques presented in this thesis will allow the nonperturbative study of topological solitons to move beyond these limitations, and explore excitations and interactions without the need for integrability or supersymmetry.

1.1.1 Formation

Topological defects relieve frustration in systems that have undergone a phase transition. For large systems (like the early universe after a grand unified theory phase transition), regions that are well-separated will remain uncorrelated during the phase transition, and inhomogeneities in the system can form; their size will be given by a length scale dependent on the details of the system and the rate of the phase transition.

The typical way in which the formation of topological defects takes place is through the Kibble-Zurek mechanism, associated with spontaneous breaking of a symmetry [85, 160, 161]. It is most successful at describing the

behaviour of phase transitions which can be described in Landau theory. During the phase transition, the order parameter can only be correlated over domains of finite size $\hat{\xi}$. These defects therefore form at the boundaries between such domains. The interaction energies of ungauged topological defects are often such that they would swiftly annihilate and would therefore be of little interest; a gauge field may be present that stabilises them, promoting the global symmetry to a local one. The reasons for this will be seen in the next chapter when we discuss Derrick’s theorem. Furthermore, if a local symmetry is broken then the density of defects is modified by the magnetic field falling out of equilibrium [75, 122].

The breaking of global symmetries to create defects by the Kibble-Zurek mechanism has been tested in the laboratory in, amongst other systems, liquid crystals [22], liquid ^4He [72] and ion chains [38]. The formation of vortices in superconducting phase transitions is an example of a situation where a local symmetry has been broken; because it is so convenient to study and yields good results, this system has been extensively tested and shown to generally¹ obey scaling predicted by Kibble-Zurek arguments [64, 101, 100, 99].

The above systems all produce defects in a rather classical manner, due to the high occupation numbers during the phase transition [139]. There is no way to be sure that this will always be the case, though, particularly in the cosmological context.

1.1.2 Quantum behaviour

While some work based on the dynamics obtained from two-particle irreducible (2PI) effective actions would seem to suggest that the deviations from classical behaviour are small [8] – at least when one considers the statistical distribution of defects – it is by no means established whether that is the case beyond next-to-leading order in 2PI, nor for gauge theories which might contain vortices or monopoles. In any case, this thesis is concerned with presenting studies of the *equilibrium* quantum behaviour of individual topological solitons; namely, their masses, excitations and interactions. While naturally this presupposes that a symmetry breaking phase

¹The author of this thesis has been involved in developing numerical simulations to study the transition to finite-size behaviour in superconducting rings; a recent discussion of this can be found in Ref. [155]

transition took place that gave rise to the defects in the first place, we are not concerned with the extent to which thermal and quantum excitations played a role close to the phase transition as defects were freezing out.

In summary, there seem to be two different questions that one can ask about how quantum behaviour would affect topological solitons: does it affect their formation, and does it change their equilibrium properties? It is the latter question which we attempt to answer in this thesis, using novel methods.

1.2 Magnetic monopoles

The earliest recorded discussion of magnetism appears to be that of the Catholic scholar Peregrinus [19, 135]. In a letter (of which Ref. [4] is a translation), he offers no speculation on the lack of isolated poles but describes the dipole as a ‘virtuous’ form bearing in itself “the likeness of the heavens”. More extensive speculation had to wait until Gilbert’s *De Magnete* of 1600 and subsequent works of the Copernican era. While the development of electrodynamics in the nineteenth century provided qualitative descriptions of the phenomena commented upon by earlier writers, it was not until the twentieth century that the literature offers us quantitative discussion on the presence – or otherwise – of monopoles.

Dirac picks up the thread in the early twentieth century [40]. Commenting on the straightforward incorporation of a magnetic monopole into quantum mechanics, he suggested that “one would be surprised if Nature had made no use of it”. A natural connection between the smallest electric and magnetic charges exists. He introduced the concept of ‘nodal lines’ (now termed *Dirac strings*), along which the phase of the quantum mechanical wave function must vanish. The conclusion is that the total magnetic flux from the endpoint of such a string would necessarily be $2\pi n\hbar c/e$, for n integer. This infers that the end of the string corresponds to a magnetic monopole, and furthermore the quantisation of electric and magnetic charge are related (in cgs units of Dirac’s original work) by

$$\frac{\hbar c}{e\mu_0} = 2, \tag{1.1}$$

as a consequence of the nodal lines being the same for any choice of wave-

function.

This observation is a direct consequence of quantum mechanics and does not depend on any inferences about particular particles that carry magnetic charge. The vector potential of a monopole can be written as

$$\mathbf{A}(\mathbf{r}) = \frac{g}{r} \frac{\mathbf{r} \times \mathbf{n}}{r - \mathbf{r} \cdot \mathbf{n}} \quad (1.2)$$

where the unit vector $\mathbf{n}$ points in the direction of the Dirac string.

The corresponding magnetic field is then the result one might anticipate for an isolated magnetic charge $\mathbf{B} = g\mathbf{r}/r^3$, except that there is a contribution $4g\pi\mathbf{n}\theta(z)\delta(x)\delta(y)$, where $\theta(z)$ is the Heaviside step function. In other words, the isolated monopole actually looks like the end of a very flexible, thin solenoid of the form studied earlier by Poincaré in Ref. [115]. He speculates on the similarity between the two objects (“Est-ce que la théorie est incomplète, parce que nous avons supposé un pôle magnétique unique . . .”) but his calculation in no way necessitates the existence of a monopole, unlike the quantum mechanical result of Dirac. We need no more than one magnetic monopole in the universe to be assured of charge quantisation, and it may be very massive and difficult to create or direct.

The next major development relevant to the work presented here comes with the work of Wu and Yang [157]. Embedding the Dirac potential in a nonabelian gauge group such as $SU(2)$ (for example, in a $U(1)$ subgroup as $A_\mu \rightarrow A_\mu \sigma^3/2$), a ‘large’ gauge transformation removes the Dirac string and leaves the gauge field

$$A_n = \epsilon_{amn} \frac{r_m}{r^2} \frac{\sigma^a}{2}; \quad (1.3)$$

essentially, the gauge transformation exactly removes the Dirac string – thanks to charge quantisation [135]. One problem, however, remains: the total colour magnetic charge remains zero. For this reason we study a model of a monopole associated with a Higgs field, turning it into a topological soliton; the symmetry breaking of the Higgs mechanism sidesteps the problems encountered when studying the gauge field alone². The resulting object – a ‘t Hooft-Polyakov monopole (first described in Refs. [145, 117]) – is discussed at length in Chapter 2. Of course, the scalar field will considerably

²Conversely, an ungauged, topologically nontrivial Higgs hedgehog configuration has divergent energy – see Section 2.2.2.

affect the classical and quantum behaviour of such a monopole – it will, for example, necessarily be massive and extended – and so finding techniques to study the behaviour and interactions of such an object is one of the aims of this thesis. Our new results concerning the 't Hooft-Polyakov monopole can be found in Chapter 8.

Alas – and despite their theoretical desirability – there have as yet been no experimental detections of magnetic monopoles despite many searches (see Refs. [58, 107] and the data tables in the latter) for production from cosmic rays, at colliders and free-floating monopoles, none have been found. Given the mass of a monopole produced at a grand unified phase transition (if there is a ‘desert’ beyond Standard Model physics up to unification) could be as high as 10^{16}GeV , this is scarcely surprising as it is not only beyond the reach of colliders, it is unlikely to be produced by processes currently taking place in the universe [121]. Nonetheless, a new experiment at the Large Hadron Collider, MoEDAL [114], is dedicated to the search for monopoles produced at the LHC (along with other exotics such as Q-balls); the more traditional experiments are also conducting searches [49]. The search therefore continues.

It is worth noting at this point that there *do* exist instances of magnetic monopoles in condensed matter systems: the ‘spin ice’ materials which have received a lot of attention in the past few years actually have monopole-antimonopole excitations, where the path between the two is marked by flipped spins that carry the excess magnetic field away – analogous to the true Dirac string [90, 50].

One last area in modern physics in which monopoles play a large role is in studies of confinement.

In Ref. [118], Polyakov studied the issue in detail in the three dimensional Georgi-Glashow model (one fewer dimension than the 't Hooft-Polyakov monopole as presented in Chapter 2), where monopole condensation takes place – seen in the lattice simulation of Ref. [33], for example. The Wilson loop operator obeys an ‘area law’ when there is a monopole gas present, characteristic of a confining phase. We will return to discuss the Wilson loop as an observable for nonabelian gauge theories in Section 4.2.3.

1.3 Quantum field theory on the computer

Carrying out physical calculations using probabilistic evaluations of integrals is an old concept, dating at least as far as the famous attempt by Lazzarini to calculate π in such a way, carrying out over three thousand trials of a “Buffon’s needle”-style experiment [108]. The idea of simulating the behaviour of an ergodic system is rather less elderly. Most historical presentations of the subject (including Refs. [132, 76]) credit the major innovations to scientists working at Los Alamos (including von Neumann, Ulam, Metropolis and Teller) in the years immediately following the Second World War. While the earliest quantitative calculations were of the statistical mechanics of interacting molecules [96], the applicability to quantum mechanical calculations had already been noted in Ref. [97].

It took a couple of decades, however, before sufficient computational capacity became available to physicists to study models of interest using these techniques. Progress was made in the 1960s studying the Ising model using both the Metropolis method [47] and a rudimentary heatbath [158]. In any case, most physics of interest at the time could be studied using analytical techniques.

However, putting a field theory on a lattice provides convenient ultraviolet and infrared cutoffs. Strong- and weak-coupling expansions were studied for lattice gauge theories by Wilson himself in his original paper [156]; the strong coupling expansion already demonstrated confinement. Yet it was only in the late 1970s that the needs of particle physics and availability of computational resources precipitated serious attempts to study nonabelian lattice gauge theories numerically.

Computer systems used for early calculations had limited memory resources and often did not handle floating-point arithmetic well (or at all). Efforts were made to cope with these issues, for example by using every bit of an integer to represent a separate spin in an Ising system [56], or approximating $SU(2)$ by a discrete subgroup [129]. These days, floating point operations can complete very quickly on dedicated hardware inside microprocessors and such low-level exploitation of processors is not quite as important.

Since the 1980s algorithms such as hybrid Monte Carlo and methods to simulate fermions on the lattice have made it possible to simulate quantum

chromodynamics with parameters close to reality. The particle spectrum and interactions of QCD are widely studied, and efforts to probe behaviour under various conditions of finite temperature and density starting to piece together the QCD phase diagram.

1.4 Summary

The aim of this thesis is to apply the powerful numerical techniques developed over the past thirty years to the study of topological solitons. While the introductory material in this chapter seeks to put these results into context, the chapters that follow explain the necessary concepts that underlie our calculations.

1.4.1 Structure of this thesis

Immediately following this Introduction, in Chapter 2 we discuss the classical properties of topological solitons. We introduce homotopy theory as a way of classifying the mappings from the vacuum manifold of a field theory into coordinate space, then go on to present the properties of the two models upon which we concentrate: the $\lambda\phi^4$ kink and the 't Hooft-Polyakov monopole.

Chapter 3 is concerned with attempts to quantise these topological defects – successfully in the case of the kink; less so for the monopole – and looks at their role in quantum theory.

Having introduced both classical and quantum properties of topological defects, we proceed to develop the techniques of lattice quantum field theory. Chapter 4 briefly recapitulates the derivation of the path integral for Euclidean quantum field theory, before going on to discretise scalar and then gauge field theory. Correlation functions and measurements are also discussed in this chapter, while Chapter 5 describes the algorithms which can be used to simulate the quantum field theories of interest in this thesis, making use of the lattice field theory developed in the previous chapter.

These four chapters provide the introductory material to the new results presented in this thesis. The following three chapters are therefore based substantially on results published in papers or submitted to a journal at the time of writing. Chapter 6 incorporates work from the paper “Quan-

tum kink and its excitations”, Ref. [124]. It uses various techniques to test the validity of the semiclassical kink results in the full quantum theory, and introduces the ‘correlator’ technique for measuring defect masses by exploiting their unique dispersion relation and finite size effects. It is followed by Chapter 7, based on results presented in paper “Soliton form factors from lattice simulations”, Ref. [125]. Here the correlator technique for measuring the mass of a defect is applied again to the $\lambda\phi^4$ model, this time at strong coupling. But the amplitude of this measurement is no longer discarded; it is used here to study the interaction between the scalar field and the kink. Ising universality is tested by comparing the measurement with exact results.

The final chapter of results, Chapter 8, applies the same techniques to the ’t Hooft-Polyakov monopole. Here there are two form factors to study, and fewer semiclassical exact results to rely on. This chapter is based on work that has been submitted to a journal for review, Ref. [126].

Our conclusions can be found in Chapter 9, as well as a short discussion of future directions.

1.4.2 Other work

In order that this thesis could be self-contained, relatively short and cogent, some work has been omitted. Two papers, Refs. [154] and [69], have not been included because the techniques used are rather different to those of lattice quantum field theory. They both rely on variational methods for finding low-lying states in Hilbert space for a quantum system (see [23] for a review of these techniques). While the tensor product states involved can be generalised to higher dimensions [150, 151], in practice it is difficult to work variationally in more than one spatial dimension.

This does not, however, mean they are irrelevant: Ref. [69] offers a way to study the ground state energies of kinks and magnons, both stationary and moving, in a way which is rather similar to that discussed in this thesis. Furthermore, the results are in infinite volume.

Several refereed conference papers were also produced, including Refs. [6] and [155]. Of these, the latter uses a Langevin simulation to study toy models of defect formation in small-volume systems to try and explain the results of Ref. [101].

A continuing affiliation with efforts to carry out high-performance computing using volunteer resources resulted in Ref. [133], a refereed conference paper presented at an applied computing conference. Further work along the same lines is in preparation. With new experiments producing more and more data, this report looks at ways of sharing the load more widely than can be done with traditional data centres. Of course, the limited bandwidth between machines in such distributed computing systems makes them poor candidates for running lattice simulations but where data analysis can be separated into many small chunks with minimal central post-processing, such techniques have been demonstrated to work well.

2 Topological defects

This chapter presents the fundamental mathematics required for the classification and study of topological defects – including solitons – at a classical level. The rest of this thesis will be concerned with the quantum properties of these extended solutions and techniques to study them.

The discussion in this chapter follows introductory material in Refs. [25, 95, 127, 152]. For the 't Hooft-Polyakov monopole, Ref. [135] was a useful resource; Ref. [106] informed the discussion on homotopy theory, while Ref. [53] provided historical context.

2.1 Classification and homotopy theory

For the time being, the discussion shall proceed in very general terms. Consider, for simplicity, an n -component real scalar field ϕ^a and potential $U(\phi)$. Suppose that a group G acts on the n -component scalar field through a matrix representation $D(g)$, $g \in G$. The assumption is that the potential (and the Lagrangian as a whole) are invariant under group transformations $D(g)$.

The minima of $U(\phi)$ yield the vacua of the theory ϕ^0 ,

$$\left. \frac{\partial U(\phi)}{\partial \phi^a} \right|_{\phi=\phi^0} = 0. \quad (2.1)$$

For each ϕ^0 there may be a subgroup H of G that leaves ϕ^0 unchanged; this is the *little group*, defined as

$$H = \{g \in G | D(g)\phi^0 = \phi^0\}. \quad (2.2)$$

The remaining elements of G act on ϕ^0 to produce different $\tilde{\phi}^0$ that are distinct minima of $U(\phi)$. The manifold of all such minima is called the *vacuum manifold* $\mathcal{M}$, which can also be thought of as the coset space G/H .

Topological defects are solutions of the field equations that are nontrivial

mappings from $\mathcal{M}$ to the physical boundary of the system; because of this, they cannot lie on the vacuum manifold everywhere inside the system – or else they could be transformed back into a trivial, constant mapping without energy cost. They are inequivalent to topologically trivial solutions, which are usually constant. A classification of the distinct, inequivalent topologically nontrivial solutions is needed; these will depend on the geometry of the boundary of the system S^{d-1} (or, rather, the asymptotic behaviour of solutions at spatial infinity) and the classification of mappings from this manifold to $\mathcal{M}$. To carry out this classification in a systematic manner, it is best to make use of some rudimentary homotopy theory.

While in algebraic topology most of the mathematics in this section is perfectly applicable to any topological space, we are interested in the case of vacuum manifolds $\mathcal{M}$ of a field theory. Therefore, the discussion has been specialised to this situation. To start with, the fundamental group $\pi_1(\mathcal{M})$ is constructed, and then the case for generalisations to higher homotopy groups $\pi_n(\mathcal{M})$ as well as the zeroth homotopy ‘group’ $\pi_0(\mathcal{M})$ can be made. It is then possible to look at different symmetry breaking patterns and say what sort of topological defects can be formed for a given vacuum manifold.

Definition Let $\mathcal{M}$ be a manifold and let $I = [0, 1]$. A continuous map $\alpha : I \rightarrow X$ is called a *path* with an initial point x_0 and end point x_1 if $\alpha(0) = x_0$ and $\alpha(1) = x_1$. If $\alpha(0) = \alpha(1) = x_0$ the path is called a *loop* with *base point* x_0 .

Definition Let $\alpha, \beta : I \rightarrow X$ be loops at x_0 . They are said to be *homotopic*, written as $\alpha \sim \beta$, if there exists a continuous map $F : I \times I \rightarrow X$ such that

$$\begin{aligned} F(s, 0) &= \alpha(s), & F(s, 1) &= \beta(s) & \forall s \in I, \\ F(0, t) &= F(1, t) = x_0 & \forall t \in I. \end{aligned} \tag{2.3}$$

The connecting map F is called a *homotopy* between α and β .

In other words, the path α can be continuously deformed into β , with the deformation parameterised by ‘time’ t . As the notation $\alpha \sim \beta$ would imply, the above definition yields an equivalence relation: the map is F is clearly symmetric and reflexive; transitivity can be shown by combining two such maps and defining a new t parameter over a rescaled unit interval.

The composition of maps lying in different homotopy classes is, under the equivalence relation of homotopy, independent of the representative of each homotopy class. Maps which are not homotopic to one another are said to fall into different *homotopy classes*.

Definition Let $\mathcal{M}$ be a manifold. The set of all homotopy classes of loops at a point $x_0 \in \mathcal{M}$ forms the *fundamental group* of $\mathcal{M}$ at x_0 , $\pi_1(\mathcal{M}, x_0)$.

The proof of the group structure can be found in textbooks such as Ref. [106]. To summarise, though, homotopies can be found that demonstrate: associativity of group elements; that an identity element exists; and that it is possible to find an inverse for any homotopy.

For a connected manifold there must exist an isomorphism between the fundamental group of loops at different x_0 , since we can continuously deform the loop accordingly. Therefore one can drop the base point x_0 and simply speak of the group $\pi_1(\mathcal{M})$.

As an example, consider the sphere S^3 , which is isomorphic to $SU(2)$. Any loop, containing however many twists, can be continuously moved over the surface of the sphere and returned to an untwisted loop which can, in turn, be shrunk to a point – much like a rubber band on a tennis ball. The fundamental group is therefore trivial, $\pi_1(S^3) = \{e\}$. By comparison, a closed loop in the unit circle S^1 (isomorphic to $U(1)$) can run from 0 to any $2n\pi$, $n \in \mathbb{Z}$. From this it can be deduced immediately that $\pi_1(S^1) = \mathbb{Z}$. Quite intuitively, this is termed the *winding number* and different homotopy classes correspond to field configurations with different winding number.

Systems where the vacuum manifold has S^1 topology commonly describe vortices. However, to obtain monopole solutions with a form like that illustrated in Figure 2.3, the vacuum manifold is typically of the form S^2 – a sphere – for which it can be shown that the fundamental group $\pi_1(S^2)$ is trivial. One is therefore compelled to generalise the construction that gave us the fundamental group from loops to spheres.

Rather than working with loops α and β parameterised by the unit interval I , consider the n -dimensional generalisation to an n -cube $I^n = I \times \cdots \times I$. Under maps α and β , it is assumed that the boundary ∂I^n is mapped to a single point, meaning that the domain of the map is an n -loop (or, more usually n -sphere) S^n . Inequivalent mappings of n -loops to the vacuum

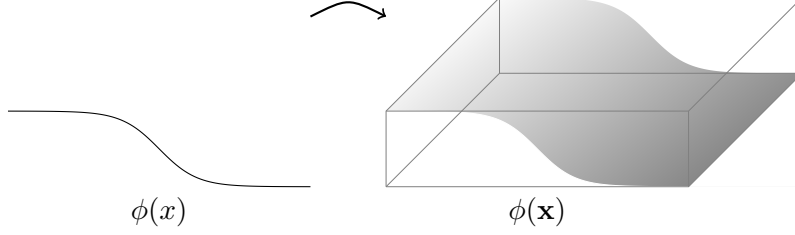


Figure 2.1: A domain wall is a kink extended into a higher dimensional system; the *codimension* is unchanged. Other topological solitons can be extended in the same way.

manifold $\mathcal{M}$ fall into separate homotopy classes, and the set of homotopy classes is called the n th. homotopy group $\pi_n(\mathcal{M})$.

By extension, $\pi_0(\mathcal{M})$ is the set of inequivalent mappings of two points (S^0) to the vacuum manifold, and is used to classify kinks and domain walls, where the vacuum manifold is discrete. It does not fall into the generalised framework given above (it is, for starters, not a group) but is a useful definition nonetheless.

Observe that kinks in $d = 1$ are a special case: the two asymptotic field values must be treated separately; the classification is the product group $\pi_0(\mathcal{M}) \times \pi_0(\mathcal{M})$ as there are mappings to two points to consider. A field theory where the vacuum consists of discrete points can then be labelled by the different choices at $\pm\infty$.

To conclude the discussion, some examples are in order. First let us observe that for an object to be of dimension D in a field theory of d spatial dimensions, it is the $(d - D + 1)$ st homotopy group that is of interest. Specifically, a topological *soliton* would be classified by $\pi_{d-1}(\mathcal{M})$, becoming a *defect* if extended into more than d spatial dimensions. A monopole in $d = 3$, a topological soliton with $d - D = 0$, would in $d = 3$ be classified by π_2 . In Chapter 8, we study it in four Euclidean dimensions, and the monopole gains a worldline but the homotopy group classifying it remains unchanged. A domain wall in $d = 3$, having dimension 2 would be classified by $\pi_0(\mathcal{M}) \times \pi_0(\mathcal{M})$ in the same number of spatial dimensions. The objects classified by $\pi_0(\mathcal{M}) \times \pi_0(\mathcal{M})$ are termed *kinks* (and are solitonic) only in $d = 1$. The relationship is illustrated in Figure 2.1.

More generally, the results are summarised in Table (2.1) for the $(3 + 1)$ -

Topological defect	Dimension	Classification
Domain walls	2	$\pi_0(\mathcal{M})$
Strings	1	$\pi_1(\mathcal{M})$
Monopoles	0	$\pi_2(\mathcal{M})$
Textures	–	$\pi_3(\mathcal{M})$

Table 2.1: The generalised homotopy groups $\pi_n(\mathcal{M})$ that can be used to carry out topological classification of important classes of defect where the system has vacuum manifold $\mathcal{M}$ in $d = 3 + 1$. Table based on material in Ref. [152].

dimensional case. In three spatial dimensions, vortices are extended into strings making them one-dimensional objects, while kinks are promoted to domain walls with dimension 2.

2.1.1 A note on moduli spaces

When one finds a minimum-energy solution (whether analytically or numerically) to a set of field equations, it is typical for there to be several parameters left undefined. Varying these parameters produces distinct solutions but does not change the energy of the system, and as a result the space of such parameters (termed moduli or collective coordinates) is termed the *moduli space*. The parameters could include the spatial co-ordinates at which a topological soliton are located.

Like the construction of homotopy theory introduced above, the term originated in algebraic geometry where it has a more general meaning.

2.2 Field theoretical models

In this thesis, we are concerned with two particular types of topological soliton, the kink and the 't Hooft-Polyakov monopole. We can demonstrate concepts and develop techniques with the kink, but we shall find that the additional complexity of the monopole means that generalisations are not always straightforward.

Here the models under study are introduced, along with the standard symmetry breaking scenarios and particle spectra. It will be seen how topological soliton solutions can be obtained. For the case of a $\lambda\phi^4$ kink, the

analysis is straightforward and can be carried out totally analytically. The situation is less simple for the 't Hooft-Polyakov monopole. Furthermore the topologically nontrivial solution of the field equations must be found numerically except in special cases.

In the previous section homotopy theory was introduced to classify the different mappings between field space and the boundary, but given some nontrivial boundary conditions how can one determine whether a stable localised solution exists? Simple scaling arguments lead to *Derrick's theorem* [39]. This involves looking at how the energy $E(a)$ of a field configuration changes under a rescaling of the co-ordinate $\mathbf{x} \rightarrow a\mathbf{x}$, noting this does not change the homotopy class to which the configuration belongs; the boundary conditions are unchanged. For theories in which $E(a)$ has no stationary point, then Derrick's theorem states that there are no static and localised solutions to the field equations.

Under the rescaling scalar fields transform trivially, $\phi(\mathbf{x}) \rightarrow \phi(a\mathbf{x})$ whereas a gauge field, being a one-form, scales as $A^\mu(\mathbf{x}) \rightarrow aA^\mu(a\mathbf{x})$. The two-form field strength $F^{\mu\nu}$ will pick up another factor of a .

For an arbitrary scalar field theory, then, in d spatial dimensions, the energy of a static configuration

$$E = \int d^d x (C(\nabla\phi(\mathbf{x}))^2 + U(\phi(\mathbf{x}))) \quad (2.4)$$

$$= E_2 + E_0 \quad (2.5)$$

rescales as

$$E(a) = \int d^d x a^{-d} (C a^2 (\nabla\phi(a\mathbf{x}))^2 + U(\phi(a\mathbf{x}))) \quad (2.6)$$

$$= a^{2-d} E_2 + a^{-d} E_0, \quad (2.7)$$

meaning that for $d > 1$ the energy is decreasing with a . Only in one dimension, then, can topological solitons of finite energy exist in a purely scalar field theory. For example the global monopole, discussed briefly in Section 2.2.2 can already be ruled out as a viable localised finite-energy configuration.

Adding a gauge field it is possible to find stationary points to the rescaling in higher dimensions; in $d = 3$ one such example is the 't Hooft-Polyakov

monopole. For $d = 4$ pure Yang-Mills possesses localised solutions termed *instantons*.

2.2.1 Kinks

The models possessing kinks with which this thesis is concerned are those with a single scalar field in $(1+1)$ spacetime dimensions. Typically the field will have a $\lambda\phi^4$ potential, but much of the following discussion only assumes that there are multiple degenerate minima to the potential.

Such a model has Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - U(\phi). \quad (2.8)$$

For a static ($\partial_0\phi = 0$) solution in such a theory, one can consider a so-called ‘virial theorem’ that causes the gradient term and the potential energy to be in balance (so long as the potential has its global minima at $U = 0$),

$$\int dx \frac{1}{2} \left(\frac{\partial\phi}{\partial x} \right)^2 = \int dx U(\phi), \quad (2.9)$$

satisfying the requirement implied by Derrick’s theorem in Eq. (2.7). This balance is necessary but not sufficient to give a minimum energy static localised configuration. Instead, returning to the equation of motion,

$$\ddot{\phi} - \nabla^2\phi = -\frac{\partial U}{\partial\phi} \quad (2.10)$$

consider static configurations $\ddot{\phi} = 0$. Then the gradient energy balances the potential energy at every point,

$$\frac{\partial\phi}{\partial x} = \pm\sqrt{2U(\phi)}. \quad (2.11)$$

This is known as the Bogomol’nyi equation for the system [12], and a solution to the field equations that also satisfies this equation is a minimum energy configuration given a choice of topological sector. It corresponds to a minimum energy for a localised configuration, saturating the *Bogomol’nyi bound* in the inequality

$$E \geq \left| \int d\phi \sqrt{2U(\phi)} \right|. \quad (2.12)$$

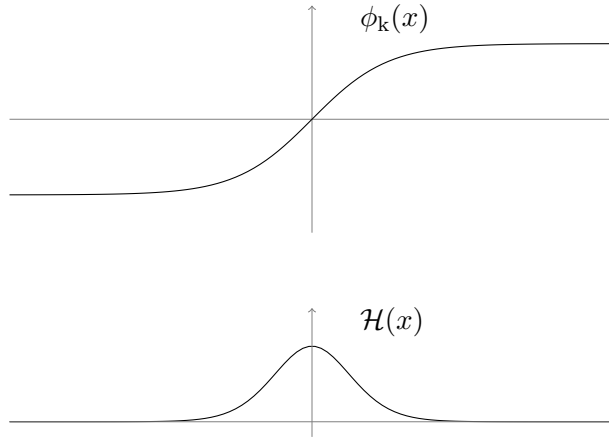


Figure 2.2: The static $\lambda\phi^4$ kink profile and the corresponding energy density.

If $U(\phi)$ is positive (and is always possible to shift a potential such that it is) then we can do the integration and obtain a superpotential $W(\phi)$ such that

$$E \geq |W(\phi(\infty)) - W(\phi(-\infty))|; \quad U(\phi) = \frac{1}{2} \left(\frac{dW(\phi)}{d\phi} \right)^2. \quad (2.13)$$

Here, the minimum energy of a localised configuration depends only on the topological sector – termed a *Bogomol’nyi bound*. The argument was first made by Bogomol’nyi in Ref. [12] (cited in Ref. [95]).

Now specialise to the case of the $\lambda\phi^4$ model and the potential

$$U(\phi) = \frac{\lambda}{4!} (\phi^2 - 6m^2/\lambda)^2 \quad (2.14)$$

$$= -\frac{m^2}{2} \phi^2 + \frac{\lambda}{4!} \phi^4 + \frac{3}{2} \frac{m^4}{\lambda} \quad (2.15)$$

where the final term on the second line makes $U(\phi)$ positive semidefinite. If one takes $m^2 > 0$, then the vacuum manifold consists of two degenerate minima of this potential for distinct $\phi = \pm m\sqrt{6/\lambda}$. The classical spectrum of this field theory is straightforward; there is a single scalar particle of mass $\sqrt{2}m$. It is immediately clear that $\pi_0(\mathcal{V}) = \mathbb{Z}_2$.

Inserting this potential in the Bogomol'nyi equation gives

$$x - x_0 = \pm \int_{\phi(x_0)}^{\phi(x)} d\phi \left(\frac{\lambda}{4!} (\phi^2 - 6m^2/\lambda)^2 \right)^{-1/2} \quad (2.16)$$

to which the solution is the static kink centred at arbitrary position x_0 (illustrated in Figure 2.2),

$$\phi_k(x) = \pm m \sqrt{\frac{6}{\lambda}} \tanh \left(\frac{m(x - x_0)}{\sqrt{2}} \right). \quad (2.17)$$

Note that the classical profile of the kink has a characteristic width given by $1/m$ (coinciding, therefore, with the correlation length in the quantum theory) and that, for large m , the solution becomes sharper and tends towards a step function. As there is only one free parameter x_0 in the solution, the moduli space of the kink is $\mathbb{R}$. This solution has energy density

$$E = \frac{1}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 + U(\phi) = 2U(\phi), \quad (2.18)$$

and integrating this result gives the classical mass

$$M = 4\sqrt{2} \frac{m^3}{\lambda}. \quad (2.19)$$

One can also define a topological charge for the system,

$$Q = \frac{\sqrt{\lambda/6}}{m} (\phi(\infty) - \phi(-\infty)). \quad (2.20)$$

Clearly, these kinks carry topological charge of ± 1 ; one can be called the kink and the other the ‘antikink’.

By studying the field configuration for two well-separated kinks of opposite charge, the interaction energy can be found. Hence, the force on a kink in the presence of another distance Δx away, is [95]

$$E_{\text{int}}(\Delta x) = -16e^{-2\sqrt{2}m\Delta x}, \quad (2.21)$$

which gives an attractive, but exponentially decaying force (that is, interestingly, independent of λ). It is, therefore, much weaker than the Coulomb force that might be expected for a pair of electrical charges. Two well-

separated kinks will take a very long time to interact.

There are many other physically interesting models which possess kinks, of which the most well-known is the sine-Gordon model [137] with potential

$$U(\phi) = \frac{m^4}{\lambda} \cos\left(\frac{\sqrt{\lambda}}{m}\phi\right). \quad (2.22)$$

Periodicities in the minima of this potential occur every $2m\pi/\sqrt{\lambda}$, and so we have $\pi_0(\mathcal{V}) = \mathbb{Z}$. There is therefore a richer spectrum of kink states present in this system, and indeed enough symmetry to make the model integrable. The techniques discussed in this thesis are general enough to apply to this model – and others – without much further work.

One can also generalise the above discussions for kinks to the case of domain walls, which are the extension of the concept into higher spatial dimensions; the vacuum manifold is unchanged.

2.2.2 Monopoles

Having discussed the general physics of monopoles in our introductory remarks, attention now turns to treating monopoles as topological solitons. It was noted before that monopoles can form when the vacuum manifold has a nontrivial second homotopy group, and we also identified that an $SU(2)$ vacuum manifold satisfied these requirements. Unfortunately, an isolated *global* monopole-antimonopole pair placed at a distance r from one another will experience a force proportional to their separation due to a linear divergence in their energies [117].

To get a stable, localised monopole solution it is necessary to look at a local symmetry breaking phase transition. At its simplest this can be $SU(2) \rightarrow U(1)$ for a system with a single Higgs field. It was in this model that 't Hooft and Polyakov studied the form of a monopole where the topologically nontrivial scalar field is stabilised by the gauge field [145, 117]. The resulting object has topological *and* magnetic charge (associated with the unbroken $U(1)$ which can be identified with electromagnetism), and is therefore often called a *magnetic monopole*.

This phase transition shall be studied in the Georgi-Glashow model of a scalar field coupled to the Yang-Mills field. With an $SU(5)$ gauge group, it was initially of physical interest as a model of grand unification [57]; in

the context of less phenomenological studies it serves as a simple model that possesses 't Hooft-Polyakov monopoles. Note, however, that all grand unified theories contain magnetic monopoles as topological solitons [121], so the discussion that follows has widespread applicability.

The model has Lagrangian density

$$\mathcal{L} = -\frac{1}{2}\text{Tr}F_{\mu\nu}F^{\mu\nu} + \text{Tr}D_\mu\Phi D^\mu\Phi - U(\Phi) \quad (2.23)$$

where $F_{\mu\nu} = F_{\mu\nu}^a T^a$ and $\Phi = \phi^a T^a$ (the adjoint representation). The co-variant derivative is

$$D_\mu\Phi = \partial_\mu\Phi + ie[A_\mu, \Phi] \quad (2.24)$$

and the field strength tensor can be written as

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ie[A_\mu, A_\nu] \quad (2.25)$$

where $A_\mu = A_\mu^a T^a$. With the chosen fields, gauge transformations are

$$\Phi(x) \rightarrow g(x)\Phi(x)g(x)^{-1} \quad (2.26)$$

$$A_\mu(x) \rightarrow g(x)A_\mu(x)g(x)^{-1} - \frac{i}{e}\partial_\mu g(x)g(x)^{-1}. \quad (2.27)$$

Much of this discussion can be generalised to higher gauge groups (of which there is a detailed discussion in Ref. [135]). For the time being, however, consider the case of $\text{SU}(2)$ where the generators obey the Lie algebra

$$[T^a, T^b] = i\epsilon_{abc}T^c \quad (2.28)$$

and we will choose to study fields in the adjoint representation of this algebra $(T^a)_{bc} = -i\epsilon_{abc}$. Taking the Higgs potential

$$U(\Phi) = -m^2\text{Tr}\Phi^2 + \lambda(\text{Tr}\Phi^2)^2, \quad (2.29)$$

the stress-energy tensor for the field theory defined by Eq. (2.23) is

$$T_{\mu\nu} = 2\text{Tr}F_{\mu\rho}F_\nu^\rho + \text{Tr}D_\mu\Phi D^\mu\Phi - \eta_{\mu\nu}\mathcal{L} \quad (2.30)$$

from which the Hamiltonian is obtained

$$H = \int d^3x T_{00} = \int d^3x \left[\frac{1}{2} (E_i^a E_i^a + B_i^a B_i^a + (D_i \phi^a)(D_i \phi^a) + \pi^a \pi^a) + V(\text{Tr} \Phi^2) \right], \quad (2.31)$$

where $\pi^a = \dot{\phi}^a$.

As with the kink, consider $m^2 > 0$. The minimum energy configuration then requires that $F_{ij} = 0$ and $D_i \Phi = 0$, and all that is needed is to minimise the Higgs potential to obtain the scalar field vacuum expectation value $\text{Tr} \Phi^2 = v^2/2 = m/(2\lambda)$. This means that the fields A_i are in a form that can be transformed everywhere to zero by a gauge transformation (‘pure gauge’), in other words

$$A_i = -\partial_i g(x) g(x)^{-1} \quad (2.32)$$

for some SU(2)-valued function $g(x)$. When this vanishes, the covariant derivative for Φ becomes an ordinary partial derivative, and so we can conclude that Φ is a constant. One can choose *unitarity gauge*, that is Φ everywhere points in a particular direction in group space, say T^3 . This breaks the SU(2) symmetry to a U(1), where transformations are group elements that satisfy

$$g(x) T^3 g(x)^{-1} = T^3. \quad (2.33)$$

Fixing this gauge for the time being, the perturbative particle content of this theory can be developed. Let

$$\Phi = (v^2 + \tilde{\Phi}) T^3, \quad A_\mu = W_\mu^1 T^1 + W_\mu^2 T^2 + a_\mu T^3. \quad (2.34)$$

The linearised $\tilde{\Phi}$ can be thought of as being massive excitations perpendicular to the S^2 vacuum manifold. Due to gauge fixing, the vacuum expectation value points in the T^3 direction. Putting the above field redefinitions into the Lagrangian and reading off the quadratic terms, the Higgs particle has mass $m_H = \sqrt{2\lambda}v$ and the two W particles have mass $m_W = gv$. The photon a_μ remains massless and is, of course, associated with the unbroken U(1) subgroup.

In summary, the vacuum expectation values lie on the surface of a vacuum

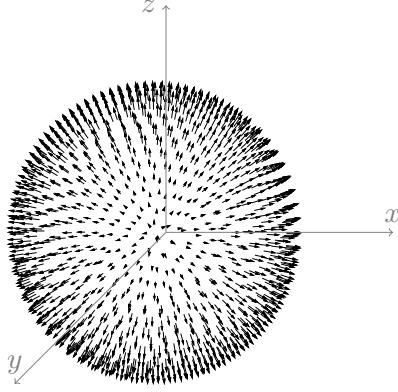


Figure 2.3: Illustration of the hedgehog Ansatz; illustration uses Ref. [70].

manifold with geometry S^2 , yielding minimum energy static configurations consistent with Φ being gauge equivalent to a constant everywhere. All the fundamental particles present in the classical formulation of this theory have been identified.

The next step will be to use the homotopy theory discussed above to deduce the distinct mappings from the vacuum manifold with topology S^2 onto the boundary of the system in $\mathbb{R}^3$ (which also happens to be S^2). Specifically, we know that $\pi_2(S^2) = \mathbb{Z}$. Different distinct mappings correspond to different winding numbers; the trivial case of a homogeneous vacuum expectation value that has just been presented clearly corresponds to zero winding number.

Any static and topologically nontrivial configurations will involve mappings from the vacuum manifold onto the boundary of the system that are not gauge equivalent to a uniform vacuum. One can imagine a solution such that the components ϕ^a of Φ point radially outwards everywhere – the ‘hedgehog’ Ansatz (see Figure 2.3)

$$\lim_{r \rightarrow \infty} \phi^a(r) = \pm \frac{vr^a}{r}. \quad (2.35)$$

These would clearly carry winding number ± 1 because a loop wound once on the spherical boundary of the system involves a single winding around the vacuum manifold. It is not possible to transform this configuration back into the trivial case $\phi^a = v$ since trying to rotate the scalar field (through a gauge transformation) to point in one direction everywhere will still leave a singularity at one point ('combing the hedgehog').

Recalling the explanation for discounting the global monopole, observe that the gradient energy of this 'hedgehog' configuration is (as stated above) linearly divergent due to the gradient term in the potential at spatial infinity. Therefore two global monopoles of opposite charge will feel a very strong attractive force. Although one can define a topological charge for such a configuration, the lack of stability is a fundamental problem with this object.

It will shortly be seen how a nontrivial gauge field configuration solves the problem of divergent gradient energy in the scalar field. Before developing the full 't Hooft-Polyakov Ansatz, some more technology is needed for the study of the residual U(1) subgroup.

To be a finite energy configuration, one requires $D_i \Phi = 0$, if not in the centre of the 'hedgehog' then certainly asymptotically far from it. Consider, then, the consequences for the gauge field

$$D_i \Phi \rightarrow 0 \quad \Rightarrow \quad \partial_i \frac{r^a}{r} - e \epsilon_{abc} A_i^b \frac{r^c}{r} \rightarrow 0 \quad \text{as } r \rightarrow \infty \quad (2.36)$$

from which one can infer

$$A_k^a(r) \rightarrow \epsilon_{ajk} \frac{r^j}{er^2} \quad \text{as } r \rightarrow \infty. \quad (2.37)$$

The corresponding magnetic field is the same as that for a Wu-Yang monopole. This is a monopole solution of the pure SU(2) field equations, when the U(1) of electromagnetism is embedded in the group and the form of an Abelian (Dirac) monopole is inserted.

The next step is to form the field tensor $\tilde{F}_{\mu\nu}$ associated with this U(1), and check that it does indeed contain this magnetic monopole as well as the massless photon in the particle spectrum discussed above.

One general form of A_μ consistent with $D_\mu \Phi = 0$ for $\text{Tr} \Phi^2 = v^2$ is

$$A_\mu^a = \frac{1}{v^2 e} \epsilon_{abc} \phi^b \partial_\mu \phi^c + \frac{1}{v} \phi^a a_\mu \quad (2.38)$$

where a_μ is a vectorial constant. As it is the only part of A_μ that remains undefined, it can be identified with the U(1) gauge potential.

Consider, as 't Hooft did in Ref. [145], a modified U(1) field strength tensor that has singularities at zeros of the Higgs field,

$$\mathcal{F}_{\mu\nu} = \hat{\phi}^a F_{\mu\nu}^a + \frac{1}{e} \epsilon_{abc} \hat{\phi}^a D_\mu \hat{\phi}^b D_\nu \hat{\phi}^c. \quad (2.39)$$

where $\hat{\phi}^a = \phi^a/v$. There are other choices (as enumerated in Ref. [62]), including the result of substituting Eq. (2.38) into the field strength tensor,

$$\mathcal{F}'_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + \frac{1}{e} \epsilon_{abc} \hat{\phi}^a \partial_\mu \hat{\phi}^b \partial_\nu \hat{\phi}^c, \quad (2.40)$$

where the principal difference is that $\mathcal{F}'$ is regular everywhere rather than having singularities at the positions of the monopoles. It is, however, Eq. (2.39) – or at least its lattice equivalent – that will be used in simulations. In either case we can obtain the full field tensor

$$F_{\mu\nu}^a = \mathcal{F}_{\mu\nu} \hat{\phi}^a. \quad (2.41)$$

All such choices must agree far from the monopole. In the topologically trivial sector, then these definitions (as well as all other possible definitions) reduce to

$$\mathcal{F}_{\mu\nu}^{\text{gf}} = \partial_\mu A_\nu^3 - \partial_\nu A_\mu^3 \quad (2.42)$$

upon choosing a constant element of Φ everywhere. Of course, it is not necessary to fix a gauge before constructing a field strength tensor for the residual U(1). Note also that it is the final term in Eq. (2.39) that behaves nontrivially in the symmetry broken phase.

Having obtained an expression for the electromagnetic field strength tensor, one can define magnetic charge. Maxwell's equations are

$$\partial^\mu \mathcal{F}_{\mu\nu} = J_\nu, \quad \partial^\mu \tilde{\mathcal{F}}_{\mu\nu} = k_\nu \quad (2.43)$$

with the definition of the electromagnetic field strength tensor given above: the right hand side of the second equation no longer vanishes. Treating it

like a current, one immediately finds

$$k_\mu = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} \partial^\nu F^{\rho\sigma} \quad (2.44)$$

$$= \frac{1}{2e} \epsilon_{\mu\nu\rho\sigma} \epsilon_{abc} \partial^\nu \hat{\phi}^a D^\rho \hat{\phi}^b D^\sigma \hat{\phi}^c. \quad (2.45)$$

Now $k_0 = \rho_M$, the magnetic charge density. We can therefore integrate k_0 to get (after integration by parts)

$$Q_M = -\frac{1}{2e} \int d^2S \epsilon_{abc} \epsilon_{\nu\rho\sigma} \hat{\phi}^a D^\rho \hat{\phi}^b D^\sigma \hat{\phi}^c \quad (2.46)$$

where the integral is over the outward normal at the spatial boundary, far from the monopole. This can only take certain values,

$$Q_M = \frac{4\pi n}{e}, \quad n \in \mathbb{Z} \quad (2.47)$$

so the conclusion is that magnetic charge is quantised.

It may be useful to note that the magnetic charge of a configuration coincides with its first Chern number [95].

With adequate definitions of the electromagnetic field strength, the magnetic charge, and having motivated the asymptotic behaviour of a ‘hedgehog’ and deduced the corresponding gauge field configuration, one can now postulate the following form for a general static monopole (the ‘t Hooft-Polyakov Ansatz)

$$\phi^a = \frac{r^a}{er^2} H(\xi), \quad A_n^a = \epsilon_{amn} \frac{r^m}{er^2} [1 - K(\xi)], \quad A_0^a = 0 \quad (2.48)$$

where $\xi = ver$ is a dimensionless variable. The boundary conditions which create a monopole (and are consistent with the scalar ‘hedgehog’ and corresponding gauge potential) are then

$$\begin{aligned} K(\xi) &\rightarrow 1, \quad H(\xi) \rightarrow 0 \quad \text{as } \xi \rightarrow 0 \\ K(\xi) &\rightarrow 0, \quad H(\xi) \rightarrow \xi \quad \text{as } \xi \rightarrow \infty. \end{aligned} \quad (2.49)$$

Solutions to the field equations that satisfy this Ansatz must be found numerically [55, 86]. Substituting minimal energy solutions back into the

Hamiltonian, the mass of a classical static monopole is found to be

$$M = \frac{4\pi v}{e} f(z) \tag{2.50}$$

where $z = \lambda/e^2$.

No solution to the field equations satisfying the asymptotic conditions given above has been found for general λ . However, the route by which we found an explicit solution for the kink was repeated for the case where $\lambda \rightarrow 0$. For this case, the derivation of the first-order Bogomol'nyi equation and solving it was carried out by Prasad and Sommerfield [120], giving the name 'BPS monopole' to the analytic solutions which occur in this case. This special case is of considerable interest, perhaps most significantly because the system of equations becomes integrable for static BPS monopoles [143].

3 Perturbative corrections to topological defects

This chapter reviews previous attempts to calculate quantum corrections to the masses of the kink and the monopole. For the kink there are consistent one-loop results, whereas there has been rather less success with the 't Hooft-Polyakov monopole. When quantising a defect by starting from the classical solution and working perturbatively, one can think of two approaches: calculating the quantum corrections to that defect, in the sense of traditional perturbative quantum field theory [31, 32, 63]; or considering the residual degrees of freedom (collective coordinates) that lie in the moduli space of the defect and quantising them [21]. The aim here is to demonstrate the limitations of these traditional approaches, and the need for the nonperturbative calculations of later chapters.

The techniques presented here have been widely applied, in both condensed matter and particle physics contexts. They were first developed by Dashen, Hasslacher and Neveu in the context of particle physics [31, 32], meaning that the quantum correction to the kink mass is often known as the ‘DHN’ result. Ohta and Kawasaki carried out calculations of interfacial tension in a ‘drumhead’ model of wetting in 1977 [109], which made use of this result (and the excitation spectrum of the corresponding Schrödinger operator) to understand interfaces in liquid-gas models.

More recently, techniques such as Zeta-function regularisation have been used [13, 15, 111]. Some recent, systematic treatments of perturbative corrections have also been carried out, such as Ref. [131].

The corrections calculated here are the result of perturbatively quantising the theory. However, these leading-order results are divergent and so renormalised perturbation theory must be used to remove divergences at the one-loop level.

3.1 General technique

This section generally reviews the discussion is found Ref. [127]. Note that, while in that source factors of $\hbar$ are included to render the order of quantum corrections unambiguous, here $\hbar$ has been set to unity, so that natural units are used throughout this thesis. Powers of λ and $\hbar$ are, as with standard quantum theory, linked together. However, the principal interest here is in terms that contribute at order λ^0 only.

Consider a scalar field ϕ in $(1 + 1)$ dimensions with action

$$S = \int d^2x \left[\frac{1}{2} (\partial_\mu \phi) (\partial^\mu \phi) - U(\phi) \right] \quad (3.1)$$

which, after integrating by parts, takes the form

$$S = \int d^2x \left[\frac{1}{2} \phi (\partial_0^2 - \nabla^2) \phi - U(\phi) \right]. \quad (3.2)$$

The next step is to find the extrema of ϕ , corresponding to static solutions ϕ_0 , which might be the trivial vacuum or a kink. Writing $\phi = \phi_0 + \delta\phi$, consider small oscillations about this minimum. Carrying out a Taylor expansion of the entries in the Lagrangian – or equivalently, working as far as second variations of the action – one obtains

$$L = \int dx \left[\frac{1}{2} \delta\phi(x) \left(-\nabla^2 + \left(\frac{d^2 U}{d\phi^2} \right)_{\phi_0} \right) \delta\phi(x) + \mathcal{O}((\delta\phi)^3) \right]. \quad (3.3)$$

The equation of motion for the small oscillations can be recognised immediately,

$$\hat{O} u_n(x) = \left[-\nabla^2 + \left(\frac{d^2 U}{d\phi^2} \right)_{\phi_0} \right] u_n(x) = \omega_n^2 u_n(x). \quad (3.4)$$

By analogy with classical mechanics, this can be called the ‘stability equation’. It is also known as the ‘auxiliary equation’ for the defect-field system. Fortuitously, it also has the form of a time-independent Schrödinger equation for excitations in the potential expanded about ϕ_0 . To find the time dependence of these small oscillations, one can take advantage of the fact

that the wave equation is separable and write

$$\delta\phi(x, t) = \phi(x, t) - \phi_0(x) \quad (3.5)$$

$$= \sum_n c_n(t) u_n(x) \quad (3.6)$$

With these redefinitions, the Lagrangian becomes

$$L = \frac{1}{2} \sum_n \dot{c}_n(t)^2 - V(\phi_0) + \frac{1}{2} \sum_n c_n(t)^2 \omega_n^2 \quad (3.7)$$

observing that here, the term $V(\phi_0)$ corresponds to the potential energy of the static field about which the expansion has been made. Except for this term, the Lagrangian now looks like a sum over a tower of harmonic oscillators in the configuration space $\{c_n\}$. Each of these oscillators can be individually quantised in the standard quantum mechanical way, and so the energy of the system will be

$$E = V[\phi_0] + \sum_n \left(N_n + \frac{1}{2} \right) \omega_n, \quad (3.8)$$

where N_n is the occupation number of the n th. state.

Two problems immediately present themselves in the above analysis. Firstly, as usual for second quantisation, it is clear that the energy E is divergent and so some form of renormalisation will be required. Furthermore, it is vital for all the ω_n in the eigenspectrum of the auxiliary equation to be nonzero or else the harmonic oscillator approximation will fail. And yet, since one would expect translational invariance from any static solution ϕ_0 , the lowest excitation will have $\omega_0 = 0$. Any true quantisation should treat it consistently but it is convenient in the following sections to ignore its effects, and sacrifice translational invariance for clarity.

The techniques of this chapter can be described as ‘semiclassical’ as they clearly depend on the background of a stationary solution to the field equations and do not fully treat the quantum corrections [31]. While the static, classical defect result is topologically nontrivial and hence not a perturbative result, the quantum corrections calculated here are just small oscillations about this result and so it should become clear that, irrespective of calculational difficulties encountered in this chapter, perturbative corrections to

static defect masses have serious limitations.

Collective coordinate quantisation (in the presentation of Ref. [21]) avoids the problem of zero modes. A static field – suppose it is a scalar field – $\phi(x)$ which describes a kink, say, can be transformed into the form $\sigma(x, X)$ where the translational invariance of the zero mode is provided by the X co-ordinate. Expansions about this solution no longer need to include the zero mode, and quantisation can proceed. While this seems like a desirable approach to follow, the results to leading order in perturbation theory (as presented here) do not differ, while higher order corrections that would otherwise diverge are not straightforward to calculate. For the monopole, discussed later in this chapter, the more fundamental problem is determining the eigenspectrum about the static monopole. Up to that step, the calculation generalises easily (as discussed in Ref. [135] and references therein).

3.1.1 Path integral approach

While the ‘DHN’ quantum correction was originally derived by the above method, it is also instructive to consider how it would be calculated in a path integral. The Minkowski space time evolution operator can be written

$$\hat{U}(T) = e^{i\hat{H}T}. \quad (3.9)$$

Applying periodic boundary conditions in the time direction, so that $\phi(x, T) = \phi(x, 0)$, one can integrate over $\phi(x, 0)$. The result can be expressed as a trace over U . Next, one applies a stationary phase approximation about some configuration ϕ_0 s. Working again as far as the second variation in the action, the path integral becomes

$$Z = e^{-S[\phi_0]} \int \mathcal{D}\delta\phi \exp\left(-i \int dx \delta\phi \hat{O} \delta\phi\right) \quad (3.10)$$

where the operator $\hat{O}$ is as defined in Eq. (3.4). Evaluating the functional determinant [112], the expression becomes

$$Z \propto e^{-iV[\phi_0]T} \left[\text{Det } \hat{O}\right]^{-1/2}. \quad (3.11)$$

There is a divergent constant prefactor that arises from evaluating the functional determinant. After some effort one obtains

$$\mathrm{Tr} [e^{-iHT}] \propto \sum_{N_n} \exp \left\{ -iT \left[V[\phi_0] + \sum_n E_n \left(N_n + \frac{1}{2} \right) \right] \right\} \quad (3.12)$$

being the same result as obtained in the previous section when $T \rightarrow \infty$.

The same calculation can be carried out for the Euclidean path integral (see Section 4.1 for a discussion). In this case, Eq. (3.11) reads

$$Z \propto e^{-V[\phi_{\mathrm{cl}}]T} \left[\mathrm{Det} \hat{O} \right]^{-1/2}. \quad (3.13)$$

and the mass can be calculated from

$$M = \lim_{T \rightarrow \infty} -\frac{1}{T} \ln \frac{Z_{\mathrm{tw}}}{Z_{\mathrm{cl}}}. \quad (3.14)$$

In doing so, the measures for the two functional determinants will cancel leaving just the correction to the classical defect mass. It is this expression that we first try to measure – albeit indirectly – in the lattice simulations of later chapters; see, for example, Eq. (8.14).

The perturbative monopole mass calculation of Ref. [88] proceeds directly from the gauge-fixed Lagrangian to the determinant result derived above albeit in Euclidean space (Ref. [87] makes use of the effective action instead). This approach has the advantage that the Faddeev-Popov gauge fixing technique can be incorporated naturally into the derivation. In the following section, the calculation for the $\lambda\phi^4$ kink is carried out using the ‘traditional’ technique of Ref. [32].

3.2 Quantum correction to the kink mass

Having developed the general technique and the potential pitfalls, specialise to the $\lambda\phi^4$ model defined in the previous chapter. Recalling the Lagrangian,

$$L = \int dx \left[\frac{1}{2}(\partial_0\phi)^2 - \frac{1}{2}(\nabla\phi)^2 + \frac{m^2}{2}\phi^2 - \frac{\lambda}{4!}\phi^4 \right], \quad (3.15)$$

it was discussed previously that when $m^2 > 0$ the field ϕ acquires a vacuum expectation value $v = m\sqrt{6/\lambda}$. There is also the topologically nontrivial

solution $v \tanh(m(x - x_0)/\sqrt{2})$. One must repeat the procedure of the previous section around these two static solutions. The two results will be divergent, and a logarithmic divergence will remain when the kink mass (the difference in energies in the two topological sectors) is obtained. This will be removed through the use of renormalised perturbation theory.

Begin by expanding about the minimum v . After integration by parts, the action has the form

$$S = \int d^2x \left[\frac{1}{2} \delta\phi(x) \left(\partial_0^2 - \frac{\partial^2}{\partial x^2} + 2m^2 \right) \delta\phi + m\sqrt{6\lambda} \delta\phi^3 + \frac{\lambda}{4!} \delta\phi^4 \right]. \quad (3.16)$$

The quadratic part of the action gives the auxiliary equation

$$\left[-\frac{\partial^2}{\partial x^2} + 2m^2 \right] c_n(x) = \omega_n^2 c_n(x) \quad (3.17)$$

with eigenfunctions $e^{ik_n x}$ and eigenvalues $(k_n^2 + 2m^2)$. The ground state is then

$$E_{\text{gs, trivial}} = \frac{1}{2} \sum_n \sqrt{k_n^2 + 2m^2} + \mathcal{O}(\lambda). \quad (3.18)$$

This is the divergent ground state energy in the symmetry broken phase that is typically removed through some sort of renormalisation, such as normal ordering. The result is exactly that obtained through second quantisation. Massive scalar particles of $\sqrt{2}m$ are manipulated by the creation and annihilation operators.

One can now do exactly the same in the presence of a static kink, and find that the auxiliary equation is given by

$$\left[-\frac{\partial}{\partial x^2} - m^2 + 3m^2 \tanh^2 \left(\frac{mx}{\sqrt{2}} \right) \right] c_n(x) = \omega_n^2 c_n(x), \quad (3.19)$$

to which the substitution $z = mx/\sqrt{2}$ is applied before solving the equation. This has the effect of scaling the solution by the kink size, making study of the eigenspectrum more straightforward.

This equation has been studied extensively, and in the context of quantum mechanics it is the Pöschl-Teller potential [119], or a special case ($n = 2$) of the Lamé equation [111]. Due to it being self-isospectral, as well as being of utility in supersymmetric quantum mechanics, it remains under study today [43]. However, for the current discussion it will be sufficient to note

that its eigenspectrum has two discrete states¹

$$c_0(z) = \text{sech}^2(z) \quad \omega_0^2 = 0 \quad (3.20)$$

$$c_1(z) = \text{sech}(z) \tanh(z) \quad \omega_1^2 = \frac{3}{2}m^2, \quad (3.21)$$

followed by the continuum of states

$$c_q(z) = e^{iqz} (3 \tanh^2(z) - 1 - q^2 - 3iq \tanh(z)). \quad (3.22)$$

The low-lying states in this spectrum can be seen in Figures 6.10 and 6.11. If the kink is placed in a box of size L with periodic boundary conditions (noting that the bound state, above, is antiperiodic), then the allowed values of q are

$$q_n = \frac{mL}{\sqrt{2}} + \delta(q_n) = 2n\pi \quad (3.23)$$

where

$$\delta(q) = -2 \tan^{-1} \frac{3q}{2 - q^2}. \quad (3.24)$$

For large z , these reduce to phase-shifted complex exponentials, just as happens when treating the system as a 1D scattering problem

$$c_q(z) \rightarrow e^{i(qz \pm \frac{1}{2}\delta(q))}. \quad (3.25)$$

Note that there exists a ‘zero mode’ $c_0(z)$ that generates translations, as well as a bound state $c_1(z)$. In Ref. [124] (the results of which are discussed in Chapter 6), we demonstrated that this state exists in the full quantum theory, and is not just an artefact of the semiclassical construction carried out in this chapter. It is also worth observing that it resembles a ‘breather mode’ of a kink-antikink pair [18], although its mass and origin are entirely different.

As was done in Eq. (3.8), a tower of harmonic oscillator states using this

¹Note that the bound state spectrum of the kink can be used to recover the original field theory and can therefore be of cosmological interest in determining the properties of topological defects formed in the early universe [149].

eigenspectrum is constructed, obtaining

$$E_{\text{gs, kink}} = V(\phi_k) + \sum_n \left(N_n + \frac{1}{2} \right) \omega_n + \mathcal{O}(\lambda) \quad (3.26)$$

$$= \frac{4\sqrt{2}m^3}{\lambda} + \frac{1}{2}\sqrt{\frac{3}{2}}m + m\frac{1}{2}\sum_n \sqrt{\frac{1}{2}q_n^2 + 2} + \mathcal{O}(\lambda), \quad (3.27)$$

since for the ground state $N_n = 0$ for all n . The kink mass and the energies of the bound states have been substituted.

As usual with second quantisation, it is possible to define creation and annihilation operators associated with each eigenmode of the auxiliary equation, and so the lowest excited state differs by energy $\omega_1 = \sqrt{3m^2/2}$. This corresponds to a quantum with eigenfunction $u_1(x)$. It is localised about the kink; the higher states pick up a phase shift due to the kink, but are not localised about it. This is one of the ways in which the interaction between ‘bulk’ particles and defects can be studied. The study of interactions between the two is a subject to which we shall return in later chapters.

Currently, the two ground state energies (with and without the kink) have divergent ground state energies which must be renormalised. Furthermore, one wants the *difference* between these two energies, as it will give the mass of the static quantum kink. This difference is calculated first, and then any remaining divergent quantities can be handled.

$$\begin{aligned} \Delta E &= E_{\text{gs, kink}} - E_{\text{gs, trivial}} \\ &= \frac{4\sqrt{2}m^3}{\lambda} + \frac{1}{2}\sqrt{\frac{3}{2}}m + \frac{1}{2}\sum_n \left[\sqrt{m^2\frac{1}{2}q_n^2 + 2m^2} - \sqrt{k_n^2 + 2m^2} \right] + \mathcal{O}(\lambda). \end{aligned} \quad (3.28)$$

Although this expression only has an ultraviolet divergence, it will be useful to reinstate the box of spatial size L into which the system was placed earlier. While it may seem counter-intuitive to put the kink and its excitations (which have asymptotic properties that would motivate antiperiodic boundary conditions) into a periodic box, the phase shift δ absorbs any such

$$\text{---} \bigcirc \text{---} + \frac{3}{2}\lambda \text{---} \times \text{---} = 0$$

Figure 3.1: The one loop self-energy graph is cancelled by the counterterm δm^2 in our calculation.

issues. The difference in energies of the scattering states then becomes

$$\begin{aligned} \frac{1}{2} \sum_n \left[\sqrt{m^2 \frac{1}{2} q_n^2 + 2m^2} - \sqrt{k_n^2 + 2m^2} \right] \\ = - \sum_n \frac{k_n \delta_n}{L} \frac{1}{\sqrt{k_n^2 + 2m^2}} + \mathcal{O}(L^{-2}) \\ \rightarrow \int dk \frac{k \delta(k)}{\sqrt{k^2 + 2m^2}} \quad L \rightarrow \infty. \end{aligned} \quad (3.29)$$

In the last line, the sum over discrete states has been turned into an integral. Furthermore, δ has been reparameterised such that

$$\delta(k) = -2 \tan^{-1} \left(\frac{3\sqrt{2}km}{2m^2 - 2k^2} \right) + \mathcal{O}(L^{-1}), \quad (3.30)$$

which can be substituted to yield

$$\begin{aligned} \Delta E = \frac{4\sqrt{2}m^3}{\lambda} + \frac{1}{2} \sqrt{\frac{3}{2}} m - \frac{3m}{\pi\sqrt{2}} \\ - \frac{6m}{4\pi\sqrt{2}} \int dp \frac{p^2 + 2}{\sqrt{p^2 + 4(p^2 + 1)}} + \mathcal{O}(\lambda) \end{aligned} \quad (3.31)$$

which is still logarithmically divergent. After all, it is the difference of two states which themselves have quadratic divergences. As this is a $1+1$ -dimensional field theory, the divergence can be removed by normal ordering or, equivalently, by the introduction of a mass counterterm.

3.2.1 Renormalisation

For a $1+1$ -dimensional quantum field theory, a one-loop divergence may be removed with a mass counterterm δm^2 . Note that it is necessary to keep the Lagrangian, the boundary conditions, and the renormalisation conditions

the same for the system with and without the kink; a common pitfall in this type of calculation is to fail to do this and therefore incorrectly remove the divergent part. Taking $m^2 \rightarrow m^2 + \delta m^2$ and rewriting the quadratic terms in the Lagrangian

$$\mathcal{L}_2 = \frac{m^2}{2}\phi^2 \rightarrow \frac{m^2}{2}\phi^2 + \frac{\delta m^2}{2}\phi^2 \quad (3.32)$$

this redefinition can be applied in turn to the Hamiltonian, to absorb the divergence in the energy of the quantum kink. The one-loop correction that is absorbed in δm^2 is then

$$\delta m^2 = \frac{3}{2}\lambda \int_{\Lambda} \frac{dp}{2\pi} \frac{1}{\sqrt{p^2 + 2m^2}}, \quad (3.33)$$

as shown in Figure 3.1.

Changing to renormalised parameters, one must add counterterms to the Hamiltonian, yielding

$$\Delta = \int dx \left[-\frac{1}{2}\delta m^2(\phi_K^2 - \phi_1^2) \right] \quad (3.34)$$

$$= \delta m^2 \frac{6m\sqrt{2}}{\lambda} \quad (3.35)$$

which will remove the logarithmic divergence. Carrying out the integral yields the famous ‘DHN’ result

$$M = \frac{4\sqrt{2}m^3}{\lambda} + m \left(\frac{1}{6}\sqrt{\frac{3}{2}} - \frac{3}{\pi\sqrt{2}} \right) + \mathcal{O}(\lambda). \quad (3.36)$$

Note that the kink profile will, of course, also change due to the renormalisation of the quadratic term in the action. It is an interesting problem to consider the limits of such ‘profile corrections’ to a quantum object, and this will be treated in a subsequent chapter. We shall argue that the form factor is the correct way to study this interaction.

3.3 Quantum correction to the monopole mass

Returning to the SU(2) Georgi-Glashow model, it is illustrative to see how much of the above technology generalises. There has, unfortunately, been

considerably less progress towards a fully consistent perturbative calculation in this situation. In this section the calculation of Kiselev and Selivanov in Ref. [88] is outlined. Their calculation is strictly interested in the terms that diverge in the limit $\lambda \rightarrow 0$ (and are thus singular in the BPS limit). Note that the perturbative correction to the kink mass only contained positive semidefinite powers of λ . The difference is due to the Coulomb potential. It is not a complete quantisation of the static monopole, merely an illustration that the BPS limit cannot be reached from the quantum monopole, since any such divergent terms are incompatible with the mass in the BPS limit being well-defined and equal to $M = 4\pi v/g$.

As the calculation is quite involved, and does not yield a result that can be easily measured (nor is central to the remainder of the thesis), only an outline of the calculation is given here with an emphasis on how the calculation differs from the kink case.

One thing to notice is that Ref. [88] studied an $\text{SO}(3)$ monopole, not its double cover $\text{SU}(2)$ that was presented in previous chapters (and will be studied on the lattice in Chapter 8). The physics is the same as far as this thesis is concerned, indeed the use of an $\text{SU}(2)$ symmetry makes the calculation resemble even more closely the combination of spin and orbital angular momenta.

3.3.1 Gauge fixing

Perhaps the most substantial difference with the kink case is that one must fix the gauge, as we did in our discussion of the classical 't Hooft-Polyakov monopole in Section 2.2.2.

The consequences of gauge fixing can be treated most easily by proceeding through the functional formalism, but it is important to note that the discussion will involve two different functional determinants, one emerging from the saddle point method and the other from fixing the gauge. The aim is to evaluate the ratio $Z_{\text{tw}}/Z_{\text{cl}}$ through the path integral

$$Z = \int \mathcal{D}A \mathcal{D}\Phi e^{i \int \mathcal{L}[A, \Phi]} \quad (3.37)$$

with and without the monopole. It is possible to use the Faddeev-Popov

method to fix the gauge [112]. This involves inserting the identity

$$1 = \int \mathcal{D}\alpha \, \delta(G) \det \left(\frac{\delta G}{\delta \alpha} \right) \quad (3.38)$$

into the path integral. Then, the original path integral becomes

$$Z = C \int \mathcal{D}A \mathcal{D}\Phi \exp \left[i \int d^4x \left(\mathcal{L}[A, \Phi] - \frac{1}{2}(G^2) \right) \right] \det \left(\frac{\delta G}{\delta \alpha} \right). \quad (3.39)$$

By exploiting the identity

$$\det \left(\frac{1}{g} \partial^\mu D_\mu \right) = \int \mathcal{D}\psi \, \mathcal{D}\bar{\psi} \exp \left[i \int d^4x \, \bar{\psi} (-\partial^\mu D_\mu) \psi \right] \quad (3.40)$$

the gauge fixing determinant can be turned into a path integral over two Grassmannian ghost fields.

3.3.2 Calculation of mass correction

Now, consider the case of a static monopole in the Georgi-Glashow model with an $\text{SO}(3)$ gauge field. The asymptotics of the field are taken to be

$$H(\xi) = \xi - 1; \quad K(\xi) = \frac{1}{\xi}; \quad \xi = \text{ver}, \quad (3.41)$$

for $r \gg 1/m_W$ in the parameterisation of Eq. (2.48).

Expanding the action of Eq. (2.23) about this asymptotic solution, letting $\phi^a \rightarrow \phi^a + \chi^a$ and $A_\mu^a \rightarrow A_\mu^a + a_\mu^a$ yields the second variation

$$\begin{aligned} \delta^2 S = \int d^4x \, & \frac{1}{2} (D_\mu a_\nu^a)^2 + \frac{1}{2} g^2 \left(\epsilon_{abc} \phi^b a_\mu^c \right)^2 + \frac{1}{2} (D_\mu \chi^a)^2 \\ & + \frac{1}{2} g^2 \left(\epsilon_{abc} \phi^b \chi^c \right)^2 + \frac{\delta^2 V}{\delta \phi^2} \delta \chi^2 + |D_\mu \psi|^2 + g^2 |\epsilon_{abc} \phi^b \psi^c|^2 \\ & + g a_\mu^a a_\nu^b \epsilon_{abc} F_{\mu\nu}^c + 2g \epsilon_{abc} a_\mu^a \chi^b D_\mu \phi^c, \end{aligned} \quad (3.42)$$

where $F_{\mu\nu}^c$ is the classical field tensor and the ghost field ψ^a arises from carrying out the nonabelian Faddeev-Popov gauge fixing procedure described above with the functional

$$G^a = D_\mu a_\mu^a + g \epsilon_{abc} \phi^b \chi^c. \quad (3.43)$$

Having just removed the determinant associated with gauge fixing with Eq (3.40), another one appears associated with the stationary phase approximation. Generalising the functional determinant result of Eq. (3.13) to the present case yields

$$Z = \int \mathcal{D}A \mathcal{D}\Phi \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S} \det H \quad (3.44)$$

and then one observes that the correction to the mass will be given by

$$\delta M = \frac{3}{2} \log \det \frac{H_{\text{tw}}}{H_C} \quad (3.45)$$

with the operators H given by

$$H_{ab} = (-D_k^2)_{ab} + g^2(\phi^2 \delta_{ab} - \phi^a \phi^b) \quad (3.46)$$

$$= [-\partial_0^2 - \nabla^2 + g^2 W^2(r) + g^2 \phi^2(r)] \delta_{ab} \quad (3.47)$$

$$+ 2\mathbf{T}_{ab} \mathbf{L} g \frac{W(r)}{r} + [g^2 W^2(r) - g^2 \phi^2(r)] \frac{r^a r^b}{r^2} \quad (3.48)$$

where $T_{ab}^i = i\sigma_{ab}^i$ and L is the standard orbital angular momentum operator. Although the potential is slightly unusual, the standard tools of spherically symmetric problems in quantum mechanics can be used. The internal SU(2) states and the angular part of the wavefunction are combined using the standard rules for the addition of angular momenta $J = L + T$. States are therefore labelled by $\mathbf{J}$ and J_3 rather than $\mathbf{L}$ and $\mathbf{T}$. Finally, one must sum over principal quantum numbers n as well as the angular momenta J to obtain the analogue of Eq. (3.8).

After much work, the correction to the monopole mass is found to have logarithmic and quadratic divergences. In contrast, the ‘DHN’ result for the kink at this stage had only a logarithmic divergence left. For the kink, a cutoff was introduced which was then removed as the final integral was finite. Kiselev and Selivanov employed Pauli-Villars regularisation to render the final result finite in their monopole calculation [110].

The final result is

$$\delta M = -\frac{m}{2\pi} \ln \frac{m_W^2}{m_H^2} + \mathcal{O}(m) \quad (3.49)$$

which is a negative correction and is (understandably) incompatible with

the BPS limit where $m_H \rightarrow 0$. A shortcut to this result would have been to expand one-loop effective potential for the scalar field

$$U_{\text{eff}}(|\Phi|^2) = \frac{3}{32\pi^2} \left[\left(\frac{4\pi^2}{3} m_W^2 e^2 m_H^2 - \frac{3}{2} \right) (e^2 |\Phi|^2 - m_W^2)^2 + e^4 (|\Phi|^2)^2 \ln \frac{e^2 |\Phi|^2}{m_W^2} - m_W^2 e^2 |\Phi|^2 + m_W^4 \right] \quad (3.50)$$

(given the renormalisation conditions $U'_{\text{eff}}(m_W^2/e^2) = 0$ and $U''_{\text{eff}}(m_W^2/e^2) = m_H^2$) around the asymptotic monopole solution [87, 135].

In conclusion, a fully consistent leading-order correction to the kink mass has been obtained. The calculation of leading-order corrections to the 't Hooft-Polyakov monopole mass has also been attempted, albeit with rather less obvious success. With the exception of the technical developments discussed at the start of this chapter for studying corrections to kink masses (and domain wall tensions), this is about as far as one can get with these semiclassical methods for studying corrections to defect masses. In the chapters that follow techniques will be presented for studying the masses of these objects nonperturbatively. There will be cause to revisit the semiclassical techniques discussed here one more time, when developing technology for the study of defect form factors; again the limitations of this approach will become clear.

4 Lattice quantum field theory

In previous chapters the classical properties of topological solitons were reviewed, followed by a discussion of various methods for quantising static soliton solutions. The aim of this thesis is to present methods for studying topological solitons nonperturbatively, and our chosen tool is lattice quantum field theory. To that end, techniques for the study of scalar and gauge fields on the lattice – both analytically and numerically – need to be introduced. The discussions follow introductory material in Refs. [29, 27, 37, 73, 102, 139].

Fermions on the lattice pose fascinating problems of their own, rather more technical than the discussions of scalar and gauge fields that will be presented here [83]. It would be interesting to study fermions coupled to topological solitons using the nonperturbative techniques under consideration, but this is left for later work.

4.1 From continuum to lattice: scalar fields

First the Euclidean path integral is reviewed which, although it was mentioned in passing in Section 3.1.1, is vital to the physics studied here. As the Euclidean path integral is real and positive definite, it can be interpreted as a probability density for a given configuration of fields in the ensemble. This interpretation is necessary if one is to simulate the field theory using the algorithms discussed later.

Furthermore, our studies of form factors in Chapters 7 and 8 depend on studying the worldline of a defect as a Euclidean quantum mechanical problem. For these reasons, the construction of the Euclidean path integral is discussed.

The standard (Minkowski) path integral for the amplitude for a particle

of mass m going from a position eigenstate $|x\rangle$ to $|x'\rangle$ is usually written [52]

$$\langle x'|U(t)|x\rangle = \int \mathcal{D}x \, e^{iS} \quad (4.1)$$

where $U(t) = e^{iHt}$ is the unitary evolution operator (as before, $\hbar = 1$). The measure is

$$\mathcal{D}x = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i a} \right)^N dx_1 \cdots dx_{N-1} \quad (4.2)$$

where the interval t is divided into infinitesimal steps $a = t/N$. In other words, Eq. (4.1) is an integral over all possible paths that start at point x and end at point x' . Different paths pick up a phase proportional to their action, which takes the form

$$S = a \sum_{n=0}^{N-1} \left[\frac{m}{2a^2} (x_{n+1} - x_n)^2 - \frac{1}{2} V(x_{n+1}) - \frac{1}{2} V(x_n) \right]. \quad (4.3)$$

This has the familiar form

$$S = \int dt \left(\frac{1}{2} m \dot{x}^2 - V(x) \right) \quad (4.4)$$

when the limit $N \rightarrow \infty$ is taken.

These expressions can be analytically continued by making the substitution $t \rightarrow it$, which means that the discretisation in the time direction must also be changed in the same way, $a \rightarrow ia$.

Now, t can be called the ‘Euclidean time’. The evolution operator becomes e^{-Ht} , which is well-defined, real and positive. The path integral can be written as

$$\langle x'|U(t)|x\rangle = \int \mathcal{D}x \, e^{-S^{\text{eucl}}} \quad (4.5)$$

where the measure is now

$$\mathcal{D}x = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi a} \right)^N dx_1 \cdots dx_{N-1} \quad (4.6)$$

and the action has become a ‘Euclidean action’,

$$S^{\text{eucl}} = iS = a \sum_{n=0}^{N-1} \left[\frac{m}{2a^2} (x_{n+1} - x_n)^2 + \frac{1}{2} V(x_{n+1}) + \frac{1}{2} V(x_n) \right]. \quad (4.7)$$

The Euclidean path integral still embodies the appropriate classical physics; the stationary phase approximation $\delta S = 0$ of the original path integral becomes a saddle point approximation of the Euclidean path integral. Different paths pick up a real and positive weight due to the Boltzmann factor containing the Euclidean action. Lastly, there is a partition function

$$Z = \text{Tr } U(T) \quad (4.8)$$

where the path integral has periodic boundary conditions (implied by the trace over all states $|x\rangle$). Setting $k_B = 1$, this gives a connection with quantum statistical mechanics for a system at a temperature $1/T$, if one notes that Eq. 4.7 coincides with the Hamiltonian for a point particle.

It is reassuring to notice how natural the discretisation is for finite N . For many-body quantum mechanical systems such path integrals can be evaluated using techniques which are generally termed *path integral Monte Carlo* (PIMC). Although the concept is similar to that of lattice field theory simulation (discussed in the next chapter), there are substantial differences in the implementation details.

Now our attention turns to the scalar field theory. The above expressions for a single particle with position operator x and corresponding eigenstate $|x\rangle$ generalise to a scalar field $\phi(x, t)$ defined at every point with corresponding eigenstates $|\phi\rangle$. The evolution operator is now

$$\langle\phi'|U(t)|\phi\rangle = \int \mathcal{D}\phi e^{-S(\phi)}; \quad (4.9)$$

the measure can be written as

$$\int \mathcal{D}x = \prod_x \left(\frac{a^{d-2}2}{\sqrt{2\pi}} \int d\phi(x) \right), \quad (4.10)$$

which clearly generalises Eq. (4.6).

Retaining the discrete time step a , one has

$$S^{\text{eucl}} = a \sum_{n=0}^{N-1} \sum_x \left[\frac{m}{2a^2} (\phi_{n+1}(x) - \phi_n(x))^2 + \frac{1}{2} V(\phi_{n+1}(x)) + \frac{1}{2} V(\phi_n(x)) \right] \quad (4.11)$$

for the Euclidean action of the field ϕ . It is possible to take the continuum limit $N \rightarrow \infty$ (and hence $a \rightarrow 0$), obtaining an action that shows manifest

Euclidean invariance,

$$S^{\text{eucl}} = \frac{1}{2}(\partial_\mu \phi)(\partial_\mu \phi) + V(\phi) \quad (4.12)$$

and indeed has the same form as the Hamiltonian for the field theory. As the metric is now Euclidean, spacetime (Greek) indices are always downstairs.

4.1.1 The scalar field on the lattice

The next step is to discretise the Euclidean action. For the sake of simplicity, consider a box of total volume $L^{d-1} \times T$ with lattice spacing a in all d directions. The derivatives in the action are replaced with forward differences

$$\partial_\mu \phi \rightarrow \frac{1}{a}(\phi(x + a\hat{\mu}) - \phi(x)) + \mathcal{O}(a^{-2}) \quad (4.13)$$

where $\hat{\mu}$ represents a unit vector in the μ direction, and the integral becomes a discrete sum,

$$\int d^d x \rightarrow a^d \sum_x. \quad (4.14)$$

Besides a factor of a^d , the polynomial terms in the action are otherwise unaffected by the discretisation.

Although other boundary conditions are discussed later in this thesis, we choose to impose periodic boundary conditions in the spatial directions for reasons of translational invariance – for the time being. A periodic box of side length L in the μ direction restricts plane waves (and hence the momenta that can be measured) to

$$p_\mu = \frac{2\pi}{L}n_\mu; \quad n_\mu = 0, 1, \dots, \frac{L}{a} - 1. \quad (4.15)$$

The discrete Fourier transform pair is taken to be

$$\mathcal{O}(\mathbf{k}; t) = \sum_{\mathbf{x}} e^{-i\mathbf{k} \cdot \mathbf{x}} \mathcal{O}(\mathbf{x}; t) \quad (4.16)$$

$$\mathcal{O}(\mathbf{x}; t) = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{x}} \mathcal{O}(\mathbf{k}; t), \quad (4.17)$$

which has the right continuum limit in large volumes.

The next thing needed is the Fourier transform of the free action. This will

permit examination of how the propagator is modified by the discretisation of the action, and thus how the dispersion relation will be changed. For the free action

$$S^{\text{eucl}} = \sum_x \left[\frac{1}{2} (\partial_\mu \phi(x))^2 + \frac{m^2}{2} \phi(x)^2 \right] \quad (4.18)$$

it is possible to carry out a discrete Fourier transform, and find

$$S(p) = m^2 + \frac{4}{a^2} \sum_\mu \sin^2 \left(\frac{ap_\mu}{2} \right), \quad (4.19)$$

the inverse of the lattice propagator $G(p)$, which has the correct continuum limit:

$$G(p) = \frac{1}{m^2 + 4a^{-2} \sum_\mu \sin^2(ap_\mu/2)} \rightarrow \frac{1}{m^2 + p^2} \text{ as } a \rightarrow 0, \quad (4.20)$$

where the last expression has the same form as the Euclidean propagator in continuum.

4.1.2 Measurements

The most obvious observables that can be measured are n -point vertex functions. Of particular importance is the two-point function, though we will also make use of four-point functions and the vacuum expectation value of scalar fields.

The discussion in this chapter focuses on systems with periodic boundary conditions and the absence, therefore, of topologically nontrivial configurations. The changes imposed on the measurement of particle states and interactions resulting from the imposition of twisted boundary conditions (and the presence of topological solitons) will be treated in subsequent chapters.

The two-point function is written in continuum as

$$\langle \phi(x_1; t_1) \phi(x_2; t_2) \rangle = \frac{1}{Z} \int \mathcal{D}\phi e^{-S[\phi]} \phi(x_1; t_1) \phi(x_2; t_2) \quad (4.21)$$

$$= \lim_{T \rightarrow \infty} \frac{\text{Tr } U(T - t) \phi(x_1) U(t) \phi(x_2)}{\text{Tr } U(T)}, \quad (4.22)$$

upon inserting energy eigenstates $|n\rangle$ and taking the limit so that the trace only has a significant contribution from the lowest-lying state, one arrives

at the spectral representation of the two-point function

$$\langle \phi(x_1; t_1) \phi(x_2; t_2) \rangle = \sum_n \langle 0 | \phi(x_1) | n \rangle \langle n | \phi(x_2) | 0 \rangle e^{-(E_n - E_0)(t_2 - t_1)} \quad (4.23)$$

which at large separations in the Euclidean time direction is dominated by the lowest energy eigenvalue E_0 , the vacuum (*not* a particle state); we therefore measure differences in energy from the vacuum. In reality, T is large but finite and so there is a contribution ‘around the world’ when measuring correlators on the lattice.

It is typical to choose to work with correlation functions of *timeslices*, which are partial Fourier transforms of the field at a given Euclidean time t , which can be written as $\phi(p, t) = \sum e^{ipx} \phi(x, t)$. If one considers the position-space field operator as creating an excitation at coordinates (x, t) , the Fourier transformed timeslice creates an excitation with momentum p at time t . Included in the linear combination of states thus created will be the single-particle momentum eigenstate $|k\rangle$. The momentum operator P and the Hamiltonian H commute, and the spectral expansion of the correlation function can be once again carried out, yielding

$$\langle \phi(t, k) \phi(0, -k) \rangle = \sum_{\alpha} \langle 0 | \phi(k) | k, \alpha \rangle \langle k, \alpha | \phi(-k) | 0 \rangle e^{-tE_{\alpha}(k)}. \quad (4.24)$$

The interpretation of this result will be central to our studies of the masses and form factors of topological solitons. The physical mass of a free scalar particle would be the lightest zero-momentum state, $m = E_0(0)$. By taking T and t large (so that the spectral expansion is dominated by the lowest energy, $E_0(k)$), the decay of the correlation function as a function of t can be measured in lattice simulations and used as a straightforward method of extracting the energies of states.

The long-distance behaviour is what one tries to measure on the lattice, but note that periodic boundary conditions will create an ‘around-the-world’ contribution to the two-point function when measured on the lattice.

4.2 Gauge fields on the lattice

In the previous section a lattice action for a single-component scalar field was formulated, and the measurements that can be carried were discussed.

Now recall the $SU(N)$ Yang-Mills action in continuum,

$$S = \int d^4x \frac{-1}{4g^2} F_{\mu\nu}^a F^{a\mu\nu}. \quad (4.25)$$

This needs to be put on a Euclidean lattice as well. In the longer term, it is necessary to know how to couple this to scalar fields – so understanding how to formulate the covariant derivative on the lattice is also necessary.

Wilson proposed an action on the lattice that was built out of plaquettes and link variables [156]. A *link variable* $U(\mathcal{P}_{xy})$ between two neighbouring lattice sites x and y is the parallel transporter associated with the path between the two sites¹. In continuum there is the formula relating

$$U(\mathcal{P}_{xy}) = P \exp \left\{ -ig \int_{\mathcal{P}_{xy}} dx_\mu A_\mu(x) \right\}. \quad (4.26)$$

For a N -dimensional complex vector ϕ , $U(\mathcal{P}_{xy})$ is an $SU(N)$ matrix that parallel transports the quantity ϕ from the vector space defined at the point y along the curve $\mathcal{P}$ to the vector space defined at the point x . Clearly, for a path of zero length, the parallel transporter is the identity; the vector space is unchanged. Two paths can be composed, namely $U(\mathcal{P}_{xz}) = U(\mathcal{P}_{xy})U(\mathcal{P}_{yz})$. Finally, reversing the path to give $U(\mathcal{P}_{yx})$ simply involves the inverse of $U(\mathcal{P}_{xy})$; for $SU(N)$ this coincides with the Hermitian conjugate of the original matrix.

Since local gauge transformations take the form

$$\phi(x) \rightarrow \phi'(x) = \Lambda^{-1}(x)\phi(x), \quad (4.27)$$

for vectors, one deduces that parallel transporters transform as

$$U(\mathcal{P}_{xy}) \rightarrow U'(\mathcal{P}_{xy}) = \Lambda^{-1}(x)U(\mathcal{P}_{xy})\Lambda(y), \quad (4.28)$$

which can be verified directly by considering the effect of gauge transformations on Eq. (4.26) when divided into infinitesimal steps.

One can now motivate and define the covariant derivative for the funda-

¹The use of U for the evolution operator and U_μ for link variables in this chapter introduces the remote possibility of confusion for which an apology is in order.

mental representation,

$$D\phi(x) = \lim_{\delta x \rightarrow 0} U^{-1}(\mathcal{P}_{x, x+\delta x})\phi(x + \delta x) - \phi(x) \quad (4.29)$$

which – as the name suggests – will transform in the same way as the field itself,

$$D'_\mu \phi'(x) = \Lambda^{-1}(x) D_\mu \phi(x). \quad (4.30)$$

Assume now that the field ϕ is defined on a lattice. The natural place for the parallel transporters is on the edges of the regular hypercubic graph linking the sites. In future, $U_\mu(x)$ will be used for the parallel transporter on the link between the site x and $x + a\hat{\mu}$. The covariant derivative becomes a finite difference and takes the form

$$D_\mu \phi(x) = \frac{1}{a} (U_\mu^\dagger(x) \phi(x + a\hat{\mu}) - \phi(x)). \quad (4.31)$$

It is therefore possible to couple a gauge field (through parallel transporters) to a scalar field on the lattice. Different representations differ in the form of the gauge-invariant coupling between the gauge and scalar fields.

Next, the action for the gauge field itself should be examined.

4.2.1 Wilson's action

Having motivated and defined the covariant derivative and the parallel transporter, one can formulate a Euclidean lattice version of the Yang-Mills action for $SU(N)$. The link variables $U_\mu(x)$ are defined on every link between lattice sites, starting at position x and pointing in direction μ . In Ref. [156], Wilson proposed considering infinitesimal closed Wilson loops involving parallel transport around squares of lattice sites. These small loops are termed plaquettes, and might be written

$$U_{\mu\nu}(x) = U_\mu(x) U_\nu(x + a\hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x). \quad (4.32)$$

Then the Wilson action takes the form

$$S = \beta \sum_{x; \mu < \nu} \left[1 - \frac{1}{N} \text{Re Tr } U_{\mu\nu}(x) \right]. \quad (4.33)$$

The relationship of β to g shall be discussed shortly. The constant term exists so that when the parallel transporters become diagonal, the action vanishes. The field strength tensor in continuum,

$$F_{\mu\nu}(x) = [D_\mu, D_\nu], \quad (4.34)$$

measures parallel transport around an infinitesimal parallelogram in the $\mu - \nu$ plane at x , it is hardly surprising that the lattice action involves plaquette operators which we have seen play a similar role. It can be shown that the Wilson action has the correct continuum limit by considering what happens to the contribution of a single plaquette $\text{Tr } U_{\mu\nu}(x)$. Using the fact that $U_\mu(x) = e^{ieaA_\mu(x)}$,

$$U_{\mu\nu}(x) = \exp(-e^2 a^2 F_{\mu\nu} - \mathcal{O}(a^3)) \quad (4.35)$$

and so

$$\text{Tr } U_{\mu\nu}(x) = \text{Tr } 1 + \frac{e^4 a^4}{2} \text{Tr } F_{\mu\nu} F_{\mu\nu} + \mathcal{O}(a^5). \quad (4.36)$$

Putting this result for the plaquette into the Wilson action of Eq. (4.33), one finds

$$S = -\beta \sum_{x; \mu < \nu} \left[1 - \frac{1}{N} \left(N + \frac{e^4 a^4}{2} \text{Tr } F_{\mu\nu} F_{\mu\nu} + \mathcal{O}(a^6) \right) \right] \quad (4.37)$$

$$= -\frac{\beta e^4}{4N} \sum_{x, \mu, \nu} a^4 \text{Tr } F_{\mu\nu} F_{\mu\nu} + \mathcal{O}(a^6), \quad (4.38)$$

from which can be read off the value of β required to agree with the Yang-Mills action when $a \rightarrow 0$,

$$\beta = \frac{2N}{g^2}. \quad (4.39)$$

It is common to set $a = 1$ in studies on the lattice; doing so here means that β itself sets the physical lattice spacing. The relationship between β and a then depends on the running of the coupling.

4.2.2 Path integral

With the above action, the partition function for pure Yang-Mills theory can be written as

$$Z = \int \mathcal{D}U e^{-S[U]}; \quad \mathcal{D}U = \prod_{x\mu} dU_\mu(x) \quad (4.40)$$

which would be expected to be gauge invariant. Since the action is invariant, the measure dU_μ should therefore itself be invariant under gauge transformations. The appropriate measure is then the Haar measure [68], which is invariant under left and right group multiplication,

$$\int dU f(U) = \int dU f(VU) = \int dU f(UV); \quad V \in G \quad (4.41)$$

and hence will be invariant under arbitrary gauge transformations $U \rightarrow \Lambda^{-1}U\Lambda$. When the Haar measure is written as an infinitesimal volume element on the group manifold, there is a free normalisation constant that is usually set such that

$$\int dU = 1. \quad (4.42)$$

It is illustrative to consider the $SU(2)$ case [102]. Taking the parameterisation of link matrices as

$$U = x_0 \mathbf{1} + ix_i \sigma^i; \quad x_0^2 + x_i^2 = 1, \quad (4.43)$$

the Haar measure can be written

$$dU = \frac{1}{\pi^2} \delta(x^2 - 1) d^4x, \quad (4.44)$$

in other words a measure with equal weight at every point on the surface of a unit 3-sphere.

For gauge theory every bit as much as the scalar field theory discussed above, it is possible to define a transfer matrix operator on the Hilbert space of states, and then demonstrate that it is a positive operator. It is also possible to rederive the partition function, as is carried out in Ref. [139]. Such calculations are involved and do not add considerably to our physical understanding of the system, and so are omitted here.

4.2.3 Measurements

When working with pure Yang-Mills theory as formulated above, the only observables that can be measured are gauge-invariant functions of link variables. These typically include plaquettes, $\text{Tr } U_{\mu\nu}$, as well as traces over larger closed loops. The *Wilson loop* is the expectation value of such a closed loop,

$$W(\mathcal{P}) = \langle \text{Tr } U(\mathcal{P}) \rangle = \frac{1}{Z} \int \mathcal{D}U \, e^{-S[U]} \text{Tr } U(\mathcal{P}), \quad (4.45)$$

where the trace *can* be taken in some representation other than the fundamental, such situations will not be considered here even though they are of some physical interest in determining whether all representations produce confining strings between quark-antiquark pairs [36].

As is known from continuum physics, the Wilson loop will obey an area law in confining phases and a perimeter law in deconfined phases. In a lattice simulation, then, it can be used as an order parameter when studying deconfinement transitions in pure gauge theories.

Just as was done for the scalar field, correlation functions can also be defined

$$G(t) = \langle \text{Tr } U(\mathcal{P}) \text{Tr } U(\mathcal{P}') \rangle - \langle \text{Tr } U(\mathcal{P}) \rangle \langle \text{Tr } U(\mathcal{P}') \rangle, \quad (4.46)$$

from which a correlation length can be obtained. These can be used to study glueballs, the fundamental particles of the pure gauge theory.

5 Simulating quantum field theories on the lattice

The previous chapter described the Euclidean path integral, and lattice regularisation. Both constructions are of utility in themselves; Euclidean quantum field theory, for example, has clear parallels with statistical mechanics. Lattice discretisation provides natural ultraviolet and infrared cut-offs; at strong coupling exact results can be obtained from high temperature expansions.

The discretisation leaves a finite (but often huge) number of lattice sites that must be integrated over in the measure. Except for the case of free field theory, such integrals cannot be done analytically so it is customary to resort to numerical evaluation of the path integral

$$\langle A \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, A \, e^{-S[\phi]}. \quad (5.1)$$

Monte Carlo integration of integrals, in general, involves the uniform sampling of random points in the region of integration [153]. While there are claims to earlier probabilistic evaluation of integrals, it was developed into an algorithmically usable state by Ulam and collaborators [132].

Considering the multidimensional integral

$$I = \int_V d^d x f(x); \quad (5.2)$$

the usual technique would be to generate N points x_n , uniformly distributed in the region V . Then, the integral can be estimated as

$$E = \frac{1}{N} \sum_{n=1}^N f(x_n). \quad (5.3)$$

For a few-dimensional integral where $f(x)$ is slowly varying and V is finite

this may be feasible. However, it is necessary to integrate over field variables at every lattice site or link; it is also known that for most parameter choices the configurations remain ‘perturbatively’ close to the classical result $\delta S = 0$. It would be far more efficient, then, to sample in a manner that takes advantage of these facts. If – instead of sampling uniformly – configurations were generated already weighted by the Boltzmann factor $e^{-S[\phi]}$, then the estimate of the expectation value $\langle A \rangle$ can be obtained by a direct average¹. This strategy is known as *importance sampling*. Typically, configurations are obtained as a sequence, and the algorithm describes the process of moving to the next configuration in the sequence with the correct weighting; this procedure is often called *updating*; one often speaks of *update algorithms*.

Importantly, this can be seen in the language of Markov processes [17]. A Markov process only knows about the previous step in the evolution of the system, so that the previous step and the next step will be independent of one another; this is the *Markov property*.

Before introducing algorithms which can carry out importance sampling for the lattice field theories defined in the previous chapter, it seems appropriate to briefly motivate and discuss some formal requirements that must be satisfied by any such algorithm.

The analogy between Euclidean quantum field theory and statistical mechanics was discussed earlier, but deserves to be revisited here. In describing how importance sampling allows us to simulate field theories, it is convenient to speak of *ensembles*. Importance sampling weighted by the Boltzmann factor $e^{-S[\phi]}$ naturally generates the canonical ensemble with zero total Noether charge (it is less trivial to look at fixed nonzero Noether charge [48]). Similarly, a microcanonical ensemble can be generated by various algorithms which do not change the action, such as classical dynamics. A grand canonical ensemble is also possible, but for many interesting field theories the weight becomes complex when a grand potential is considered rather than the action, leading to an infamous sign problem [113].

¹For clarity, throughout this chapter ϕ is used to represent any collection of dynamical scalar and gauge fields, with the appropriate measure in the path integral. The conjugate momenta to these fields will be denoted π . In many cases these will be treated as vectors, so that $\pi^2 = \sum_x \pi(x)^2$. The use of π for the conjugate momentum means that Q has been chosen for the invariant distribution of the process – even though π is commonly used – to avoid confusion.

Concentrating on the canonical ensemble, consider the distribution $Q[\phi]$ of configurations ϕ in the path integral and also transition probabilities between states $P[\phi \rightarrow \phi']$. The transition probabilities between any two states can be thought of as lying in a large matrix.

With this language, the requirements are

- *Strong ergodicity*, which is a statement that although importance sampling is used, no region of configuration space is explicitly excluded from our sampling algorithm; the transition probability between any two configurations is always nonzero:

$$P[\phi \rightarrow \phi'] > 0. \quad (5.4)$$

This condition is also known as the *irreducibility* of the Markov chain.

- *Detailed balance*, a statement that the canonical ensemble is in equilibrium on the microscopic scale as well as the macroscopic:

$$P[\phi \rightarrow \phi']Q[\phi] = P[\phi' \rightarrow \phi]Q[\phi'], \quad (5.5)$$

which implies the result

$$\sum_{\phi'} P[\phi \rightarrow \phi']Q[\phi] = Q[\phi']. \quad (5.6)$$

This is essentially the statement that the distribution Q in the canonical ensemble is necessarily an eigenvector of the transition matrix P [130]. While detailed balance is therefore a stronger requirement, it has perhaps a more physical interpretation. In any case, many simulational algorithms satisfy Eq.(5.5), even though Eq.(5.6) is sufficient for a canonical ensemble.

5.1 Algorithms

The *Metropolis algorithm* can be stated as follows [93].

1. Given some initial configuration ϕ , a random change is made to create a proposed new configuration ϕ' .
2. The change in the Euclidean action $\Delta S = S[\phi'] - S[\phi]$ is calculated. If the action is decreased, the proposed configuration is accepted. If the

action is increased, the proposal is accepted with probability equal to $e^{-\Delta S}$. More formally, the acceptance probability is

$$P_{\text{acc}}[\phi \rightarrow \phi'] = \min \left\{ 1, \frac{Q[\phi']}{Q[\phi]} \right\}. \quad (5.7)$$

As formulated, strong ergodicity is clearly satisfied. Usually, however, the change is only made to one lattice site or link variable – and it is typically a rather small change. These practicalities mean that a single update step no longer satisfies the strong ergodicity condition. Instead, it is possible to consider a sequence of single update steps and argue that many such steps taken together will allow strong ergodicity to be satisfied.

For detailed balance, assume (without loss of generality) that the ‘forward’ transition from ϕ to ϕ' reduces the action. Then one has, almost by inspection, satisfied Eq. (5.5)

$$P[\phi \rightarrow \phi']Q[\phi'] = 1 \cdot Q[\phi]. \quad (5.8)$$

It is not necessary to calculate the action for the whole lattice when the update step occurs; it suffices to look at neighbouring sites or all the plaquettes to which the current link contributes (known as ‘staples’, and illustrated in Figure 5.1). Typically the updates will be carried out by choosing sites or links throughout the lattice in a systematic manner; it is common to use a ‘checkerboard’ strategy so that updates take place independently of each other (and thus do not depend on recomputation of the contribution to the action from neighbours or staples), as shown in Figure 5.2. It is straightforward to parallelise such an update step with domain decomposition methods.

Unsurprisingly many variations on the same basic idea are possible. Those which are relevant to the discussion here include:

- *Multi-hit* algorithms or *improved Metropolis*. If the recalculation of the contribution to the action is computationally costly one can repeat the Metropolis update step for a particular site several times in one visit. In the limit of infinite repeated update steps per site, this becomes the **heatbath algorithm** [28].
- *Parallel tempering* or *replica exchange* [144]. A series of simulations

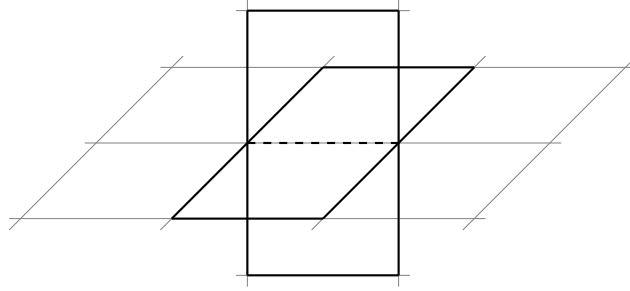


Figure 5.1: Visualisation of the links that contribute to a ‘staple’ for three dimensional lattice gauge theory. The plaquettes highlighted in bold must be recalculated to determine the change in the action due to updating the dashed link.

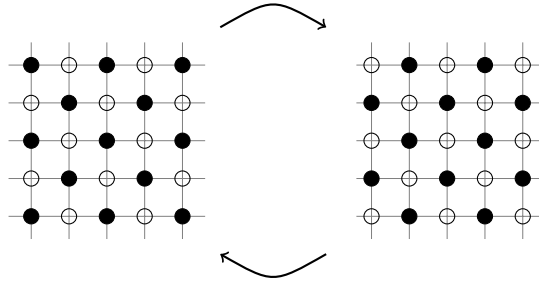


Figure 5.2: The checkerboard update concept, illustrated for a 2D scalar field. Half the sites are updated simultaneously on an alternating basis. The technique can be generalised to gauge theories in a straightforward manner.

are carried out simultaneously with actions differing only by the choice of some parameter g . If the spacing $\Delta g = g - g'$ between the different parameter choices is sufficiently small then a Metropolis-style update step which exchanges the two simulations may have a reasonably large transition probability. The process should be compared with the histogram techniques discussed later in this chapter; both techniques are due to Swendsen and collaborators.

5.1.1 Hybrid Monte Carlo

When introducing the Metropolis algorithm above, it was noted that small update steps are preferred (typically changing a single site or link at a time) to increase acceptance rates and thus improve efficiency of the algorithm. Physically, it is also likely that small fluctuations from the classical vacuum contribute more to the path integral; there is no benefit to importance sampling if large nonlocal changes are attempted at each step because the acceptance probability is likely to be vanishingly small. Therefore, standard Metropolis updates change the field configuration in a rather diffusive manner.

One can reformulate the problem as a Hamiltonian system that adds conjugate momenta, turning the Euclidean action into a ‘potential’,

$$\int \mathcal{D}\phi A[\phi] e^{-S[\phi]} = C \int \mathcal{D}\pi \mathcal{D}\phi A[\phi] e^{-\frac{1}{2}\pi^2 - S[\phi]} \quad (5.9)$$

with the momentum field π conjugate to ϕ (regardless of whether ϕ is scalar, gauge or fermionic) [42, 84]. Evolution with this Hamiltonian is in a new, fictitious, computer time τ . The constant of integration C results from the Gaussian integration of the momenta, which will cancel with the same factor from the partition function in any calculation. One can then consider the molecular dynamics evolution resulting from numerically integrating Hamilton’s equations,

$$\dot{\pi} = -\frac{\delta S[\phi]}{\delta \phi} \quad (5.10)$$

$$\dot{\phi} = \pi, \quad (5.11)$$

which are integrated from the initial configuration $\{\phi, \pi\}$ to a final config-

uration denoted $\{\phi', \pi'\}$.

For a good choice of symplectic integrator [92], numerical evaluation of these equations preserves the Hamiltonian, and is reversible. Furthermore, the evolution is area-preserving, namely

$$\det \left(\frac{\partial \{\phi', \pi'\}}{\partial \{\phi, \pi\}} \right) = 1 \quad (5.12)$$

so the measure is unchanged by the evolution.

Evolving with a symplectic (molecular dynamics) algorithm would generate a microcanonical ensemble so long as one is careful to handle errors from the discrete time step. Such an algorithm would not be ergodic on its own. Instead, one uses numerical evolution of the equations of motion as the basis for an algorithm which takes advantage of the Gaussian contribution to the action of the conjugate momenta:

1. Generate the additional momentum field (or fields) π with probability distribution $P_G[\pi] \propto e^{-\pi^2/2}$.
2. Evolve the configuration and momenta by integrating Hamilton's equations for some time τ with a symplectic algorithm.
3. Carry out an accept-reject step on the change in the Hamiltonian. Specifically, if the Hamiltonian is decreased then the new configuration ϕ' is accepted unconditionally; if the Hamiltonian is increased then the new configuration is accepted with probability equal to ratio of the Boltzmann factors $e^{-H[\pi', \phi'] + H[\pi, \phi]}$. The momenta are then discarded.

As expressed here, the acceptance probability can be written as

$$P_{\text{acc}}[\{\pi, \phi\} \rightarrow \{\pi', \phi'\}] = \min \left\{ 1, \frac{e^{-H[\pi', \phi']}}{e^{-H[\pi, \phi]}} \right\}. \quad (5.13)$$

Carrying out an accept-reject step on the Hamiltonian rather than the action is sufficient to generate a canonical ensemble $Q[\phi] = e^{-S[\phi]}$, because detailed balance is satisfied [42]. Clearly $Q[\phi]P_G[\pi] \propto e^{-H[\pi, \phi]}$, so

$$\begin{aligned} Q[\phi]P_G[\pi]P_{\text{acc}}[\{\pi, \phi\} \rightarrow \{\pi', \phi'\}] \\ &= Q[\phi']P_G[\pi']P_{\text{acc}}[\{\pi', \phi'\} \rightarrow \{\pi, \phi\}] \\ &= Q[\phi']P_G[-\pi']P_{\text{acc}}[\{\pi', -\phi'\} \rightarrow \{\pi, -\phi\}] \end{aligned} \quad (5.14)$$

since $H[\pi, \phi] = H[-\pi, \phi]$. The measure $\mathcal{D}\pi \mathcal{D}\pi'$ is also invariant. With these facts in mind, the statement of detailed balance

$$\begin{aligned} \int \mathcal{D}\pi \mathcal{D}\pi' Q[\phi] P_G[\pi] P_{\text{acc}}[\{\pi, \phi\} \rightarrow \{\pi', \phi'\}] \\ \int \mathcal{D}\pi \mathcal{D}\pi' Q[\phi'] P_G[-\pi'] P_{\text{acc}}[\{\pi', -\phi'\} \rightarrow \{\pi, -\phi\}] \end{aligned} \quad (5.15)$$

follows immediately. Furthermore, the accept-reject step is required solely as a consequence of the Hamiltonian only being approximately conserved by the molecular dynamics algorithm, or else the above equations simplify.

5.2 Measurements and statistics

Having discussed how to simulate a field theory on the lattice, it is necessary to understand better how to carry out measurements based on the configurations generated by our simulations. The expectation value $\langle A \rangle$ is represented as a path integral by

$$\langle A \rangle = \frac{1}{Z} \int \mathcal{D}\phi e^{-S[\phi]} A[\phi]; \quad Z = \int \mathcal{D}\phi e^{-S[\phi]} \quad (5.16)$$

It was noted in the previous chapter that the path integral is still valid for the lattice discretised Euclidean quantum field theory. The configurations generated by the algorithms in the previous section are sampled weighted by the Boltzmann factor $e^{-S[\phi]}$. From this, it is reasonable to assume that calculating the sample mean $\bar{A}$ of $A[\phi]$ by averaging over such configurations will give us an estimator of the true value $\langle A \rangle$. If N configurations are generated, labelled ϕ_n , clearly

$$\bar{A} = \frac{1}{N} \sum_n A_n \quad (5.17)$$

where $A_n = A[\phi_n]$.

5.2.1 The histogram method

Naturally, importance sampling makes it easy to calculate estimates of expectation values for observables when the action of the theory being simulated is the same as the theory for which one wants to carry out mea-

surements. Yet there is a method, first discussed by Ferrenberg and Swendsen [51], of using the sample distribution of A (which, by construction above, has been obtained) to yield information about A for different parameter choices than those used in the simulation. This is frequently of use when looking at the behaviour of observables in the vicinity of the phase transition, or to check that the two ensembles under consideration are truly at equilibrium.

Supposing the Euclidean action has a parameter g with associated term $A[\phi]$, which may include hopping terms. Then, by inspection of the path integral, the probability density of A can be written

$$P(A|g) = \frac{1}{\tilde{Z}(g)} N(A) e^{-gA}, \quad \tilde{Z}(g) = \sum_A N(A) e^{-gA}, \quad (5.18)$$

where $N(A)$ is the number of configurations where the measurement lies in the interval $(A, A + dA)$. Therefore, the histogram of values A at parameter g approximates the true probability distribution at A . It is then possible to use the same sample but with a different weighting; consider some parameter choice g' such that $g - g'$ is sufficiently small. Then the probability distribution at g' is given by

$$P(A[\phi] | g') = \frac{P(A[\phi] | g) e^{-(g'-g)A[\phi]}}{\sum_{A[\phi]} P(A[\phi] | g) e^{-(g'-g)A[\phi]}}; \quad (5.19)$$

as no other parameter in the Euclidean action is changed. This result can be seen as ‘correcting’ for the difference in weights in the importance sampling between the actual parameters at which the simulation was carried out and desired parameters for which results are required. For the same reason, the distance in parameter space must be kept relatively small so that the statistics remain adequate.

This technique, in summary, amounts to an indirect attempt to reconstruct the partition function over a range of parameters using a single simulation. Other, similar techniques will be used when studying defect masses and are discussed in subsequent chapters.

5.2.2 Autocorrelation of samples

It was mentioned above that successive configurations generated by any usefully efficient simulation algorithm will tend to be correlated. This is even true of Hybrid Monte Carlo; otherwise transition probabilities would be low and computer time would be wasted by generating configurations that were not used. Therefore, some effort must be made to understand the extent to which successive measurements are correlated, and how many updates must be made between measurements before one can consider them to be independent.

Using the generic quantity A again, it is possible to define an autocorrelation between measurements in the sequence as

$$C_A(\tau) = (A_n A_{n+\tau}) = \langle A_n A_{n+\tau} \rangle - \langle A \rangle^2 \quad (5.20)$$

and the normalised autocorrelation for separation τ is then

$$\rho_A(\tau) = \frac{C_A(\tau)}{C_A(0)}. \quad (5.21)$$

The autocorrelations $C_A(\tau)$ decay with increasing τ , at a rate that depends on various factors including the choice of update algorithm and the observable A . Normally, the sample standard deviation s is obtained through

$$s^2 = \overline{A^2} - \bar{A}^2, \quad (5.22)$$

and the standard error of the mean (the deviation of the estimated mean from the true mean) can be estimated as $s_M = s/\sqrt{N-1}$. However, the autocorrelation means that the assumption of independence underlying the sampling of A is invalid, and there are fewer than N independent measurements in the sample. With this in mind, the standard deviation can be written

$$s_{\text{decorrel}}^2 = \frac{1}{N^2} \sum_{n,m=1}^N C_A(n-m). \quad (5.23)$$

One can estimate the *exponential autocorrelation time* for A $\tau_{A,exp}$ from the decay of $C_A(\tau)$. For large τ one will typically find

$$C_A(\tau) \sim e^{-\tau/\tau_{A,exp}}; \quad (5.24)$$

one typically reserves the label τ_{exp} for the exponential autocorrelation time of the observable with the longest autocorrelation time; depending on the update algorithm, it may be infinite [140].

The above definitions should be contrasted with the *integrated autocorrelation time* $\tau_{A,int}$ obtained by considering the behaviour of the true variance estimate above in the limit $N \rightarrow \infty$. By identifying the number of independent measurements from the limiting result, one obtains

$$s_{\text{deccorrel}}^2 \rightarrow (\overline{A^2} - \overline{A}^2) \frac{2\tau_{A,int}}{N}; \quad \text{where} \quad \tau_{A,int} = \frac{1}{2} \sum_{\tau=-\infty}^{\infty} \rho_A(\tau). \quad (5.25)$$

The conclusion is that skipping about $2\tau_{A,int}$ measurements should yield an independent sample.

Furthermore, it is known that $\tau_{A,int} \leq \tau_{A,exp}$. Simply put, $\tau_{A,int}$ gives exactly how many measurements in a large sample are independent, while $\tau_{A,exp}$ provides an upper bound, a conservative but easy to calculate estimate of the autocorrelation.

The autocorrelation $C_A(\tau)$ is particularly easy to calculate using the Wiener-Khinchin theorem [71]. This states that the power spectrum and the autocorrelation form a Fourier transform pair, namely

$$\sum_{\tau=0}^{N-1} C_A(\tau) e^{-2\pi i \omega \tau / N} = \left| \sum_{n=0}^{N-1} A_n e^{-2\pi i \omega n / N} \right|^2 \quad (5.26)$$

with the availability of fast Fourier transforms, this may be the most efficient way to rapidly estimate the autocorrelation time of an update process so long as there are enough samples that the periodicity has a negligible effect.

It is very important to note that different observables can have radically different autocorrelation times. Depending on the difficulty of measurement or available storage space it may not be desirable to store every possible measurement of the observable during a simulation. Then an estimate of the autocorrelation time can be made and used to work out an appropriate measurement spacing.

5.2.3 Initialising a simulation

When a simulation is started from scratch, it is almost certain to begin from a configuration which does not lie in the canonical ensemble, unless one uses

a configuration which was taken from the end of a previous simulation run. Specifically, one can think of ‘hot’ and ‘cold’ starts, depending on whether the lattice sites or links are initialised randomly or uniformly to a fixed value respectively [102, 140, 141].

Luckily, Eq. (5.6) codifying detailed balance implies that convergence to the canonical ensemble is assured [102]. Applying the transition matrix corresponding to the chosen update method repeatedly will eventually generate the canonical ensemble,

$$\lim_{n \rightarrow \infty} P^n Q_0[\phi] = Q[\phi] \quad (5.27)$$

where the ‘distribution’ corresponding to the initial configuration shall be denoted $Q_0[\phi]$.

The only requirement is that the canonical ensemble $Q[\phi]$ and the initial configuration $Q_0[\phi]$ are not orthogonal, and this is assured by strong ergodicity. Unfortunately, there is no guarantee that this convergence will take place quickly, or indeed at the same rate for all observables. If it is possible to measure the exponential autocorrelation time then that can be used to estimate the deviation from equilibrium, but all too often it is necessary to rely on empirical observations that our measurements are no longer biased by our initial configuration.

A related issue is *metastability*, where the system remains stuck in a state which is long-lived but may actually be irrelevant to the canonical ensemble. Without accurate knowledge of the exponential autocorrelation time for all observables, it is not possible to be sure that a given run is free from metastability.

The classic scenario in which metastability occurs is when two phases are at coexistence near a first-order phase transition; a simulation seeing only one of the two phases will yield incorrect results. A more pertinent example is, for the topological solitons under study in this thesis, systems with long-lived defect-antidefect pairs. The dynamics of the theory will eventually annihilate this pair (or create others) but with only finite computer time available, the signal can come to dominate measurements. As a result, great care must be taken in thermalising a system to avoid undesirable metastability.

Finally, a few words are in order on how to determine whether a simulation

functions as intended. Some are fairly trivial: the acceptance rate can be tuned and checked for a Metropolis algorithm, while for hybrid Monte Carlo a useful test is that the ensemble average of the error in the molecular dynamics step is close to zero, namely

$$1 = \left\langle e^{-(H[\pi', \phi'] - H[\pi, \phi])} \right\rangle \geq e^{-\langle H[\pi', \phi'] - H[\pi, \phi] \rangle}. \quad (5.28)$$

Beyond algorithmic correctness there are other, more physical approaches to verifying the implementation of an algorithm. To check that the results of a simulation are valid, comparison can be made with work in the literature, especially where histograms of observables have been provided. As an example pertinent to Chapter 8, Ref. [81] contains histograms of measurements of observables for the 3D Yang-Mills system with adjoint Higgs field, which were compared to those obtained by the code written to calculate results for this thesis (as applied to a 3D system with periodic boundary conditions).

5.2.4 Critical slowing down

When one tries to look at the continuum limit, or in the vicinity of any other second order phase transition, the correlation length ξ (related to the inverse of the mass scale) diverges. When ξ is much larger than the lattice spacing, more updates will be required to decorrelate an observable as each configuration is correlated on a larger scale. The effect is known as *critical slowing down*, and like the Kibble-Zurek mechanism (which also involves restrictions on the propagation of signals as a phase transition is approached) outlined in the introduction a dynamical scaling law is satisfied,

$$\tau_{int,A} \propto \xi^{z(A)}. \quad (5.29)$$

The exponent z , can be reduced by careful choice of algorithm; the worst-performing are typically Metropolis implementations where a single site or link is changed at a time which yields $z \gtrsim 2$. If it is assumed that local fluctuations introduced by Metropolis updates carry out random walks on the lattice [141], after n updates, the typical distance over which the fluctuation has had influence is $\sqrt{n}$; to decorrelate over distance ξ will therefore take ξ^2 steps; therefore $\tau \approx \xi^2$.

5.2.5 The jackknife and bootstrap: resampling methods

In the previous section a true estimate of the error in the mean was constructed, given a sequence of measurements of an observable. This section is concerned with how to obtain error estimates for derived quantities (such as fit parameters) or where the sampled data are, for some reason, subject to bias. An obvious example is the measurement of a correlation function – perhaps the timeslice correlator

$$\langle \phi(t, -k) \phi(0, k) \rangle \propto \left(e^{-E(K)t} + e^{-E(k)(T-t)} \right); \quad T \gg t \gg 0. \quad (5.30)$$

The mass of a state is often obtained by fitting this expression at long distances to the expected exponential form. Normally, the data points in a fit are independent of each other. Of course, the measurement of the timeslice correlation function at different distances is itself correlated!

Various techniques have been developed specifically to treat this problem [98], but here instead it is instructive to consider a class of more general statistical techniques known as resampling (and not to be confused with the histogram reweighting discussed above). These techniques reduce the bias in estimates of quantities by repeatedly generating new samples from the initial set of data and looking at the behaviour of a set of such samples.

Suppose a least-squares fit of Eq. (5.30) is carried out. In a standard least-squares fitting scenario, the error in the fit parameters is estimated by assuming that the residuals come from the deviation of *independent* measurements from the fit curve. The sum of these residuals then follows a χ^2 distribution, and the error in the fit parameters can be calculated.

If the data are not independent, then the error estimated in the fit by the standard method will be incorrect. Resampling methods offer a general framework for tackling this problem, and similar issues in other circumstances where the error in a quantity is difficult to estimate.

Two resampling methods for finding estimators of quantities of interest are in use; the *jackknife* and the *bootstrap*. Both are based on an initial set of independently and identically distributed data $\{A_n\} = A[\phi_n]$, $n = 1, \dots, N$ (these might be the decorrelated results obtained from sampling at appropriate spacings as discussed previously). New samples are then computed from this set, and estimators of the true (unbiased) result can then be obtained based on the variability of these new samples.

Helpfully, the jackknife can be applied to the nonlinear least squares fitting problem in a manner that has been shown to remain valid when the data in the fit are not independent (in other words, *robust to heteroscedasticity*). When studying correlation functions, this is frequently the case.

The jackknife was originally used as a way of estimating bias in an estimator $\hat{g}(A_1, \dots, A_N)$ of a quantity by recalculating the estimator for every subset of data which has one item deleted, which shall be denoted $\hat{g}_i$. This new calculation removes the first-order term in the bias. Furthermore, it was later argued (in Ref. [147]) that the $\hat{g}_i$ can be treated as independent and identically distributed (with reduced bias than $\hat{g}$), and furthermore the set $\{\hat{g}_i\}$ has error $\sqrt{N(N-1)}$ times that of $\hat{g}$. Indeed, where $\bar{g}$ is the mean $\bar{A}$, these assumptions can be shown to be exact. Motivated by this, the jackknife estimator of variance is defined as

$$s_{\text{jack}}^2 = \frac{N-1}{N} \sum_{i=1}^N \left(\hat{g}_i - \frac{1}{N} \sum_{j=1}^N \hat{g}_j \right)^2. \quad (5.31)$$

The jackknife is computationally intensive, but only uses N resamplings and does not depend on a source of random numbers. By contrast, the *bootstrap* can use more than N samples from the data. Each new sample is obtained by sampling with replacement from the original set $\{A_n\}$ to give $\{A_n^*\}$, one then computes the estimator $\hat{g}_n^*$ from this new sample. This is repeated for B different samplings with replacement which will, for most data sets, only be a very small fraction of the possible permutations; as the true bootstrap estimator depends on the estimator for all conceivable permutations, this constitutes a Monte Carlo procedure to approximate the bootstrap estimator. The variance is then approximated by

$$s_{\text{boot}}^2 = \frac{1}{B} \sum_{m=1}^B \left(\hat{g}_m^* - \frac{1}{B} \sum_{n=1}^B \hat{g}_n^* \right)^2 \quad (5.32)$$

which coincides with the theoretical definition of the bootstrap in the limit $B \rightarrow \infty$. The jackknife and the bootstrap are, clearly, closely related. The bootstrap is computationally more intensive, but is more versatile; however, exact results about the reliability of resampling techniques in certain situations will lead us to also use the jackknife.

Indeed, for the purposes of this thesis it would be useful to apply the above general approach to a nonlinear fit to data, and so the standard method for applying the jackknife technique to nonlinear least squares fits merits discussion here. Having measured data points (perhaps of timeslice correlators) (x_i, y_i) with $i = 1, \dots, N$, the fit would be to a nonlinear model with parameters g ,

$$y_i = f(x_i, g) + \epsilon_i. \quad (5.33)$$

Here, f is a given function, the x_i are known exactly and the ϵ_i are the residuals. For example, x_i could be the separation and y_i the measured timeslice correlation at the given separation – the parameters g would then be the amplitude and mass. Assume – for the time being – that the ϵ_i are independent and identically distributed. The least squares fit is carried out to obtain an estimator $\hat{g}$, which if the ϵ_i have a Gaussian distribution happens to be the optimal estimator.

Now, consider the set of (x_i, y_i) with one data point j deleted at a time; the estimator of g obtained by fitting to this resampled set being denoted $\hat{g}_j$. The jackknife estimator of the error in g is then

$$s_{\text{Jack}}^2 = \frac{N-1}{N} \sum_{j=1}^N \left(\hat{g}_j - \frac{1}{N} \sum_{j=1}^N \hat{g} \right)^2. \quad (5.34)$$

While nonlinear least squares fitting algorithms can be computationally expensive, and so generating N estimates of g could take a while, it is possible to accelerate the process if one uses the fit parameters from the previous resample for the next iteration.

Helpfully, while the above result is predicated on independent and identically distributed residuals ϵ_i , if the variance of each residual is not identical then the estimate of the variance from the jackknife can still be trusted.

6 Quantum kink and its excitations

This chapter is based on research originally presented in Ref. [124], which was carried out in collaboration with my supervisor Arttu Rajantie. Changes to the format of equations, tables and graphs have been carried out. The method and results are as presented in that paper, and additional explanatory material has been added as well as references to the introductory material of previous chapters.

As we saw in Chapters 2 and 3, the $\lambda\phi^4$ kink is a useful ‘toy model’ for the study of topological solitons, both classically and in the quantum theory. It was for this reason that our first attempts to study the excitations and interactions of topological solitons used this model. This chapter, and the next, both demonstrate the techniques we developed using this model; Chapter 8 uses these techniques in the rather more sophisticated context of a ’t Hooft-Polyakov monopole.

6.1 Introduction

There has been widespread interest in the excitation spectra of topological defects, although mostly as a calculational tool for finding perturbative corrections to the mass of the defect [2, 9, 32, 88, 89, 105, 111, 127]; we saw details of such calculations in Chapter 3. However, excitations themselves are of physical interest [21, 63, 77]. Bound states of point-like defects correspond to new particle species, and in the case of extended defects they would be particles propagating on the brane. For instance, in braneworld models all the standard model particles can be thought of as states localised on a domain wall [44]. Finding stable particles localised on defects in fully non-perturbative approaches would therefore correspond to completely new particle species; indeed, for strongly-coupled theories there is no a priori

reason to expect that the perturbative spectrum is accurate. The bound states of cosmic strings have been previously studied as a potential way of stabilising string loops [66, 65, 149]. In some sense, reconstructing the excitation spectrum is the opposite approach to that taken classically in Vachaspati’s paper on the reconstruction of a field theory [148].

In this chapter we present the results of our investigations of field correlation functions in the presence of a kink; we make use of the techniques of lattice Monte Carlo simulation discussed in Chapters 4 and 5. Our approach bears some similarity with Refs. [21, 63, 77], in that we are considering the quantum behaviour of soliton excitations. We show that the correlators can be used to measure non-perturbatively the mass of the kink and its excitation spectrum. Furthermore, we obtain approximate wavefunctions for the excitations based on Monte Carlo data. Previously these have only been studied at the linear level.

Previous work has measured the kink mass with ‘Kadanoff’s non-local operator’ [24]; but more generally, the mass of topological defects has usually been calculated on the lattice by finding the free energy of the defect [16, 74, 80, 123]. This is taken as the difference in free energy between the system with the defect present, and the same system but without the defect. The defect is often created using twisted boundary conditions, so one is effectively measuring the response to that twist [67]. Since the partition function cannot be determined by Monte Carlo simulations, one must measure derivatives of the mass and then perform finite differencing from a point where the mass is known. Typically, this is at a phase transition which is where the errors in Monte Carlo simulations are at their largest (due to critical slowing down, discussed in Section 5.2.4).

The method of calculating the kink mass we propose requires study only of a topologically nontrivial sector, and only at one parameter choice. This gives a check on errors which may be present in the ‘twist’ method. It may also serve to reduce the amount of calculation required since it only requires Monte Carlo simulations to be carried out for the desired parameters.

We expect that these techniques can be generalised to more sophisticated defects such as monopoles (treated in Chapter 8); the extension to domain walls is relatively trivial.

6.1.1 The $\lambda\phi^4$ model

Kinks, or their higher dimensional counterparts domain walls, can occur where the vacuum manifold after spontaneous symmetry breaking is not simply connected, and the field can take on a different vacuum expectation value in different parts of the space. Domain walls could have formed in the early universe due to random fluctuations leading to different patches of space occupying different, disconnected vacua.

In this paper, we focus on kinks in a $1 + 1$ -dimensional model. We will review the necessary details from Chapter 2 here. The Lagrangian has the form of Eq. (2.8)

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \phi)^2 - U(\phi) \quad (6.1)$$

with the potential of Eq. (2.15),

$$U(\phi) = -\frac{m^2}{2!}\phi^2 + \frac{\lambda}{4!}\phi^4 + \frac{3}{2}\frac{m^4}{\lambda}. \quad (6.2)$$

In the classical broken phase, we will have $m^2 > 0$. The vacuum is then $\phi_0 = \pm m\sqrt{6/\lambda}$. In $(1 + 1)$ dimensions, the dimensionless parameter that appears in perturbative results will be λ/m^2 .

A kink configuration interpolates between the two vacua. We can create a topological kink by requiring that $\phi \rightarrow \phi_0$ as $x \rightarrow +\infty$ and $\phi \rightarrow -\phi_0$ as $x \rightarrow -\infty$, with one choice of sign being termed a ‘kink’ and the other an ‘antikink’. The kink solution is obtained via the Bogomol’nyi equation for the kink [12, 127],

$$\frac{\partial \phi}{\partial x} = \pm \sqrt{2U(\phi)}. \quad (6.3)$$

The static classical kink solution ϕ_k is a minimum-energy configuration satisfying Eq. (6.3) that interpolates between the two vacua in the broken phase. In the frame of the kink,

$$\phi_k(x, t) = m\sqrt{\frac{6}{\lambda}} \tanh\left(\frac{mx}{\sqrt{2}}\right). \quad (6.4)$$

The classical mass M_{cl} is, from integrating the energy density,

$$M_{\text{cl}} = 4\sqrt{2}\frac{m^3}{\lambda}. \quad (6.5)$$

6.1.2 Bound and scattering states

We wish to consider the excitation spectrum in the presence of a kink. A more complete discussion can be found in Section 3.2. We expand about the classical kink solution, $\phi = \phi_k + \hat{\phi}$ and eliminate terms using the equation of motion. We must solve the auxiliary equation to obtain the form of the excitations about the defect. This has the form of a Schrödinger equation with a Pöschl-Teller potential,

$$\left[-\frac{\partial^2}{\partial x^2} + 3m^2 \tanh^2 \frac{mx}{\sqrt{2}} - m^2 \right] c_n(x) = E_n c_n(x) \quad (6.6)$$

and eigenfunctions

$$c_0(x) = \cosh^{-2} \left(\frac{mx}{\sqrt{2}} \right) \quad (6.7)$$

$$c_1(x) = \cosh^{-2} \left(\frac{mx}{\sqrt{2}} \right) \sinh \left(\frac{mx}{\sqrt{2}} \right) \quad (6.8)$$

$$c_q(x) = e^{\frac{iqmx}{\sqrt{2}}} \left[3 \tanh^2 \left(\frac{mx}{\sqrt{2}} \right) - 1 - q^2 - 3iq \tanh \left(\frac{mx}{\sqrt{2}} \right) \right] \quad (6.9)$$

and corresponding energy eigenvalues

$$E_0 = 0 \quad (6.10)$$

$$E_1 = m \sqrt{\frac{3}{2}} \quad (6.11)$$

$$E_q = m \sqrt{\frac{q^2}{2} + 2}. \quad (6.12)$$

E_0 corresponds to a Goldstone mode that shifts the kink in the x -direction; E_1 corresponds to a massive localised ‘bound state’ and E_q are a continuum of scattering states labelled by $-\infty < q < \infty$. We impose antiperiodic boundary conditions on a box of length L with $L \rightarrow \infty$. Then, the following expression for the allowed parameters q can be found, based on odd integer multiples of π/L plus a phase shift due to the kink

$$q_{n,\text{ant}} \frac{mL}{\sqrt{2}} = (2n+1)\pi + \delta(q_{n,\text{ant}}); \quad n = 0, 1, 2, \dots \quad (6.13)$$

where $\delta(q)$ is the phase shift experienced by particles scattered off the kink [127],

$$\delta(q_n) = -2 \tan^{-1} \frac{3q_n}{2 - q_n^2}. \quad (6.14)$$

The allowed values merge into a continuum when $L \gg 1/m$. Thus, in the infinite volume limit, the ratio of the bound state energy to that of the lowest-energy scattering state is $\sqrt{3/4} = 0.866 \dots$

6.2 Quantum kink mass

In this section we review existing approaches to calculating the kink mass. One can calculate the leading quantum correction to the classical kink mass in the weak-coupling limit $\lambda/m^2 \ll 1$ analytically by summing up the zero-point energy contributions from all the excitations (6.10-6.12). This corresponds to one-loop level in perturbation theory, and gives [32]

$$M_{\text{1loop}} = M_{\text{cl}} + m \left[\frac{1}{6} \sqrt{\frac{3}{2}} - \frac{3}{\pi\sqrt{2}} + \mathcal{O}(\lambda/m^2) \right]. \quad (6.15)$$

We reviewed the details of this calculation in Chapter 3. The result has recently been generalised to finite volume in Refs. [105, 111].

A non-perturbative alternative is to consider the response of the system to a ‘twist’ by carrying out lattice simulations [67]. The mass of a topological defect can be calculated from the difference between the free energy F_{tw} in the topologically nontrivial sector containing the defect (in this case a kink), and the free energy F_0 in the topologically trivial sector,

$$\Delta F = F_{\text{tw}} - F_0 = -\log \frac{Z_{\text{tw}}}{Z_0}. \quad (6.16)$$

Then we have

$$M_{\text{k}} = \lim_{T \rightarrow \infty} \frac{\Delta F}{T}, \quad (6.17)$$

where T is the length of the system in the time direction. Unfortunately Eq. (6.16) is impossible to measure in Monte Carlo simulations because one only samples the partition function. We therefore resort to calculating

derivatives of this mass with respect to a parameter g in the Lagrangian:

$$\frac{\partial \Delta F}{\partial g} = \left[\left\langle \frac{\partial S}{\partial g} \right\rangle_{\text{tw}} - \left\langle \frac{\partial S}{\partial g} \right\rangle_0 \right]. \quad (6.18)$$

One then integrates this expression from a location where the mass of the defect is known exactly, such as the phase transition where the kink mass vanishes. In this paper we will take parameter $g = m^2$, and then Eq. (6.18) becomes

$$\frac{\partial \Delta F}{\partial m^2} = \frac{L}{2} [\langle \phi^2 \rangle_{\text{tw}} - \langle \phi^2 \rangle_0] \quad (6.19)$$

where L is the spatial system size.

Unfortunately, linear error propagation is not very reliable for estimating the error in this integral; indeed, if we add more points this will tend to *increase* the error without any justifiable cause. One must also consider the error resulting from the quadrature. In practice, errors in the kink free energy are under better control if one uses finite differences [123]; error propagation can then use the standard linearised results. We have then

$$\Delta F(m_2^2) - \Delta F(m_1^2) = -\ln \frac{\left\langle e^{-\frac{1}{2}(m_2^2 - m_1^2) \sum_x \phi^2} \right\rangle_{m_1^2, \text{tw}}}{\left\langle e^{-\frac{1}{2}(m_2^2 - m_1^2) \sum_x \phi^2} \right\rangle_{m_1^2, 0}}, \quad (6.20)$$

a formula which resembles the ‘resampling’ technique of Ferrenberg and Swendsen introduced in the previous chapter (and originally proposed in Ref. [51]). Indeed, one way of checking that the measurement spacing is appropriate is to check that the measurements for the change of ΔF from m_1^2 to m_2^2 are the same when taken from above or below.

An equivalent criterion, applicable to Eq. (6.19), is to actually use the ‘resampling’ method to ensure that neighbouring values of $\langle \phi^2 \rangle$ agree under the shift of m^2 . Unfortunately, this does not remove the problem with propagation of errors. This is a topic that we shall revisit in our analysis of the ’t Hooft-Polyakov monopole mass in Chapter 8.

One of the main drawbacks of this approach is the requirement to numerically integrate (or take finite differences) from, for example, the phase transition. Close to the phase transition, the errors in the expectation values in Eq. (6.19) will be quite large due to critical slowing down. Worse, the overall error in the kink mass will increase with the length of the integration

path. A local calculation of the mass of a topological defect will give better control of the errors and provide a check on the results obtained by the traditional approach.

One other alternative way of carrying out the twist should be mentioned here. Noting that the twisted boundary conditions can be rewritten as a change to the action, we can instead opt to parameterise this contribution and vary it from an ‘untwisted’ to ‘twisted’ situation incrementally. This has been used in, for example, Ref. [35, 82].

6.3 Correlation functions

In this section we consider correlation functions in the topologically non-trivial sector. Specifically, we will work with two- and four-point functions of the scalar field. We use the two-point functions to study the kink mass, and the four-point functions to study the kink spectrum. These approaches are motivated by the spectral expansion of the field in the presence of a kink.

6.3.1 Spectral expansion

Recalling Eq. (4.23), the correlation function of general operators $\mathcal{O}_i(t)$ localised in time has a spectral expansion

$$C_{ij}(t_2 - t_1) = \langle \mathcal{O}_i(t_1) \mathcal{O}_j(t_2) \rangle = \sum_{\alpha=0}^{\infty} \langle 0 | \mathcal{O}_i | \alpha \rangle \langle \alpha | \mathcal{O}_j | 0 \rangle e^{-(t_2-t_1)E_\alpha} \quad (6.21)$$

where $|0\rangle$ is the ground state of the relevant topological sector and $|\alpha\rangle$ are a complete set of states with energies E_α . By a suitable choice of operators, we can determine individual terms in this expansion. By calculating the corresponding correlator in the presence of a kink, we can therefore determine its complete excitation spectrum, at least in principle.

In practice, the energies E_α can be determined either by a straightforward fit to Eq. (6.21) or by using the ‘Lüscher-Wolff’ method [20, 61, 94]. In the latter approach, we consider the generalised eigenvalue problem

$$C_{ij}(t)\rho^{(n)} = \lambda_n(t, t_0)C_{ij}(t_0)\rho^{(n)} \quad (6.22)$$

where the eigenvalues λ_n have the long-distance behaviour $\lambda_n(t) = e^{-tE_n}$ as $t \rightarrow \infty$. The energies are then obtained with

$$E_n = \log \left(\frac{\lambda_n(t, t_0)}{\lambda_n(t+1, t_0)} \right). \quad (6.23)$$

We show in Sections 6.3.2 and 6.3.3 that by considering operators $\mathcal{O}_i$ constructed from one or two field operators ϕ , we can measure not only the excitation spectrum in the rest mass of the kink, which corresponds to the linearised results in Eqs. (6.10-6.12), but also approximate wave functions of these states and the mass of the kink itself.

6.3.2 Two-point function

Let us first consider operators $\mathcal{O}_k = \phi(k) = \int dx e^{ikx} \phi(x)$ for different momenta k , which are quantised because of the antiperiodic boundary conditions,

$$k = \frac{(2n+1)\pi}{L}. \quad (6.24)$$

Momentum conservation requires the momenta of the two operators to be equal, so for each momentum k we have the correlation function

$$C(t_2 - t_1; k) = \int_{x_1} \int_{x_2} dx_1 dx_2 e^{ik(x_1 - x_2)} \langle \phi(x_1, t_1) \phi(x_2, t_2) \rangle \quad (6.25)$$

as calculated in our Monte Carlo simulation for the kink sector of the broken phase. This has a spectral expansion

$$C(t_2 - t_1; k) = \sum_{\alpha=1}^{\infty} \langle 0 | \phi(t_1; k) | \alpha \rangle \langle \alpha | \phi(t_2; -k) | 0 \rangle e^{-(t_2 - t_1)E_\alpha}. \quad (6.26)$$

Because of momentum conservation, all states $|\alpha\rangle$ in this expansion must have overall momentum k . The lightest such state corresponds to the boosted kink. Other states in the expansion correspond to excited states of the kink and two-particle states consisting of a kink and a scalar particle. In the limit $k \ll m$, there should be a significant gap between the energies; the correlator Eq. (6.25) is therefore dominated by the boosted kink at long time separation $t_2 - t_1$. By analogy with the eigenspectrum given in Section

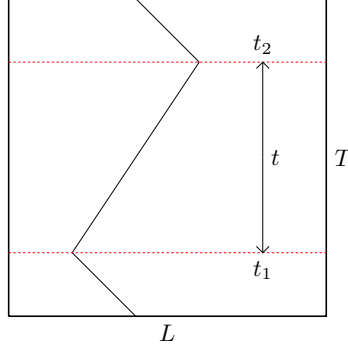


Figure 6.1: Schematic picture of ‘recoil’ behaviour at a classical level. The kink is forced to match up due to periodic boundary conditions in the time direction (of length T). It receives a kick from the scalar particle at t_1 which, to conserve momentum, it must give up at $t_2 = t_1 + t$.

6.1.2, we expect

$$\begin{aligned}
C(t_2 - t_1; k) = & \langle 0 | \phi(t_1; k) | \text{kink}_k \rangle \langle \text{kink}_k | \phi(t_2; -k) | 0 \rangle e^{-(t_2 - t_1) E_k^{\text{kink}}} \\
& + \langle 0 | \phi(t_1; k) | \text{bs} \rangle \langle \text{bs} | \phi(t_2; -k) | 0 \rangle e^{-(t_2 - t_1) E_k^{\text{bs}}} \\
& + \sum_{\alpha=1}^{\infty} \langle 0 | \phi(t_1; k) | \alpha \rangle \langle \alpha | \phi(t_2; -k) | 0 \rangle e^{-(t_2 - t_1) E_{\alpha, k}^{\text{bulk}}} \quad (6.27)
\end{aligned}$$

where E_k^{kink} is the energy of a boosted kink with momentum k ; E_k^{bs} and $E_{\alpha, k}^{\text{bulk}}$ are the energies for the bound state and a scattering state (a particle in the bulk) respectively. This spectrum has only one massive bound state, but we do not rely on this assumption in the calculations which follow. It is momentum conservation and the long-distance behaviour of the moving kink state that allow us to distinguish between the states when carrying out a fit to measurements.

The physical interpretation of Eq. (6.27) is that the dominant contribution to the correlator comes from the ϕ particle created at t_1 absorbed by the kink before re-emerging to be annihilated at t_2 . Not only must momentum be conserved by this process, but we also impose periodicity in the time direction: $\phi(x, t) = \phi(x, T + t)$. As long as $k \ll m$ and $(t_2 - t_1) \gg 1/m$, the kink width is small relative to other relevant length scales, we can treat the kink as a point particle. Close to the phase transition, m approaches

zero and the kink width diverges, and lower momenta k and longer time separations have to be used.

Consider the action of a point particle of mass M in free space whose momentum increases by k at t_1 and decreases by k at $t_2 = t_1 + t$. Periodic boundary conditions in the Euclidean time direction of size T require that the initial and final x -components of the velocity must match. Then,

$$S = M \left[t \sqrt{1 + v_1^2} + (T - t) \sqrt{1 + v_0^2} \right] \quad (6.28)$$

noting that the corresponding velocities v_0 and v_1 are related by $t \leftrightarrow (T - t)$. We assume that the kink moves non-relativistically, so $v_0, v_1 \ll 1$ and obtain

$$S \approx M \left[T + \frac{1}{2} v_1^2 t + \frac{1}{2} v_0^2 (T - t) \right] \quad (6.29)$$

and, by applying the stationary phase approximation we expect to see a dominant contribution to the correlation function, as measured on the lattice, that has the form

$$C(t; k) \sim \exp \left[-\frac{1}{2} \frac{k^2}{M} \frac{t(T - t)}{T} \right]. \quad (6.30)$$

We have assumed that the interaction between the scalar particle and the kink is trivial and independent of the change in the momentum. This is not necessarily the case. In particular the situation when $k \sim M$ means that the form factor affects the shape of the correlator. We will return to this in the following chapter. In the infinite-time limit, $T \rightarrow \infty$, Eq. (6.30) reduces to the non-relativistic kinetic energy of a particle with momentum k [63]. In practice, the finite T effects are important, and therefore we keep the equation in this form. By fitting the asymptotic long-time behaviour of the correlator Eq. (6.25) to Eq. (6.30), we can determine the kink mass M because the momentum k is fixed. This gives us a direct way of measuring the kink mass.

6.3.3 Four-point functions and excitation spectrum

To find the excitation spectrum in the rest frame of the kink, we need to use operators with zero overall momentum. Therefore we consider two-particle operators which correspond to creating two particles on a timeslice,

separated by distance¹ Δx

$$\mathcal{O}_{\Delta x}(t) = \sum_x \phi(x, t) \phi(x + \Delta x, t). \quad (6.31)$$

We can use the Lüscher-Wolff method of Eq. (6.23) to determine the energy spectrum $\{E_\alpha\}$, which now includes only states in the rest frame of the kink and should therefore correspond directly to the negative parity states in Eqs. (6.10-6.12). Whether a given state is a localised bound state of the kink or a free particle state can be determined by investigating its dependence on the volume L . In the infinite-volume limit, free particle states should behave as

$$E^2 \sim m^2 + k^2 = m^2 + \frac{(2n+1)^2 \pi^2}{L^2} + O(L^{-4}). \quad (6.32)$$

In contrast, a localised bound state would have an exponentially small finite-size effect. When the volume L is smaller than the inverse mass $1/m$ we would expect the kink to be ‘squeezed’ and the bound state to have lower energy.

The other way of seeing the localisation of the first state is to try to reconstruct the wavefunctions from the generalised eigenvectors of Eq. (6.22). We can then compare our results with the eigenfunctions of the fluctuation field in the presence of a continuum kink given by Eq. (6.6), or its discrete equivalent discussed later.

Using (6.21) to rewrite the generalised eigenvalue problem (6.22)

$$\begin{aligned} \sum_l \langle 0 | \mathcal{O}_{\Delta x} | l \rangle e^{-E_l t} \sum_{\Delta y} \langle l | \mathcal{O}_{\Delta y} | 0 \rangle \rho_{\Delta y}^{(n)} \\ = \lambda_n \sum_m \langle 0 | \mathcal{O}_{\Delta x} | m \rangle \sum_{\Delta z} \langle m | \mathcal{O}_{\Delta z} | 0 \rangle \rho_{\Delta z}^{(n)}, \end{aligned} \quad (6.33)$$

we expect $\lambda_n(t) = e^{-tE_n}$ at long distance and so

$$\sum_{\Delta y} \langle m | \mathcal{O}_{\Delta y} | 0 \rangle \rho_{\Delta y}^{(n)} = \delta_{mn} \quad (6.34)$$

is a reasonable ansatz. Using our choice of two-particle operators this be-

¹One could also work with Fourier-transformed fields with appropriate antiperiodic momenta.

comes

$$\sum_y \sum_{\Delta y} \langle m | \phi(y) \phi(y + \Delta y) | 0 \rangle \rho_{\Delta y}^{(n)} = \delta_{mn}. \quad (6.35)$$

We now split the field ϕ into the kink background ϕ_k and fluctuations $\hat{\phi}$. We are in the broken phase; we assume in our expansion that the one-particle states are well-separated from the two-particle states. Then for the one-particle states

$$\sum_y \sum_{\Delta y} \langle m | [\phi_k(y + \Delta y) + \phi_k(y - \Delta y)] \hat{\phi}(y) | 0 \rangle \rho_{\Delta y}^{(n)} = \delta_{mn}. \quad (6.36)$$

We further assume that the field $\hat{\phi}$ can be decomposed into orthogonal modes – the wavefunctions for each energy eigenstate. Noting that this means

$$\sum_x \hat{\phi}_m(x) \hat{\phi}_n(x) = \delta_{mn} \quad (6.37)$$

we identify

$$\hat{\phi}_n(x) = \sum_{\Delta x} \rho_{\Delta x}^{(n)} [\phi_k(x + \Delta x) + \phi_k(x - \Delta x)]. \quad (6.38)$$

This shows that, for one-particle states, the convolution of the generalised eigenvectors $\rho^{(n)}$ of the correlation matrices $C(t)$, $C(t_0)$ with the kink background gives the wavefunction. A starting assumption for the form of the kink background in the weak-coupling limit is that it takes the standard shape of Eq. (6.4) but with the renormalised mass taking the place of m . This can be obtained from simulations with periodic boundary conditions.

6.4 Numerical calculations and simulations

For calculations on a lattice of size $L \times T$, we make the standard choice of discretisation. The Euclidean action is

$$S = \sum_{\mathbf{x}} \left[- \sum_{\mu=1}^2 \phi(\mathbf{x}) \phi(\mathbf{x} + a\hat{\mu}) + a^2 \left(2 + \frac{m^2}{2} \right) \phi(\mathbf{x})^2 + a^2 \frac{\lambda}{4!} \phi(\mathbf{x})^4 \right] \quad (6.39)$$

where the summation over $\mathbf{x}$ runs over all sites, and $\hat{\mu}$ is a unit vector in either direction on the lattice; compare with Eq. (4.18). For the remainder

of this paper, we have set $a = 1$, and instead vary λ and m^2 .

Periodic boundary conditions are employed in the time direction at all times. The topologically nontrivial sector, where the kink is present, is simulated by imposing antiperiodic boundary conditions on the lattice in the spatial direction.

Finite lattice spacing changes the dispersion relation by introducing a momentum cutoff. For a free particle the dispersion relation is that of Eq. (4.19), namely

$$E(k) = \sqrt{\frac{4}{a^2} \sin^2 \frac{ak}{2} + m^2}. \quad (6.40)$$

This modifies the $O(L^{-4})$ contribution in Eq. (6.32).

6.4.1 Linearised calculations

The linearised energy spectrum in Eqs. (6.10-6.12) is calculated in continuum, and to be able to compare it with our Monte Carlo results, which are obtained on a discrete lattice, we need to understand what effect the discretisation itself has. We can see this by considering the Schrödinger problem for a kink in discrete space.

A straightforward way of understanding the finite-size and discretisation effects is to solve the lattice Schrödinger equation for a kink background. Splitting ϕ into kink background ϕ_k and fluctuations $\hat{\phi}$ as before, we find the classical discrete kink by the gradient flow method,

$$\begin{aligned} \phi_k(x, \tau + \delta\tau) = \phi_k(x, \tau) - \delta\tau & \left[2\phi_k(x, \tau) - \phi_k(x + a, \tau) - \right. \\ & \left. - \phi_k(x - a, \tau) - m^2\phi_k(x, \tau) + \frac{\lambda}{3!} (\phi_k(x, \tau))^3 \right] \end{aligned} \quad (6.41)$$

where antiperiodic boundary conditions are used and $\delta\tau$ is chosen to give good convergence. The eigenvectors and eigenvalues of $\hat{\phi}$ are then obtained by solving

$$\left[D^2 - \frac{m^2}{2} 1 + \frac{\lambda}{4} B \right] c_n(x) = E^2 c_n(x) \quad (6.42)$$

where D^2 is the second-order lattice derivative with antiperiodic boundary conditions, and B is the diagonal matrix with entries $B_{xx} = \phi_k(x)^2$.

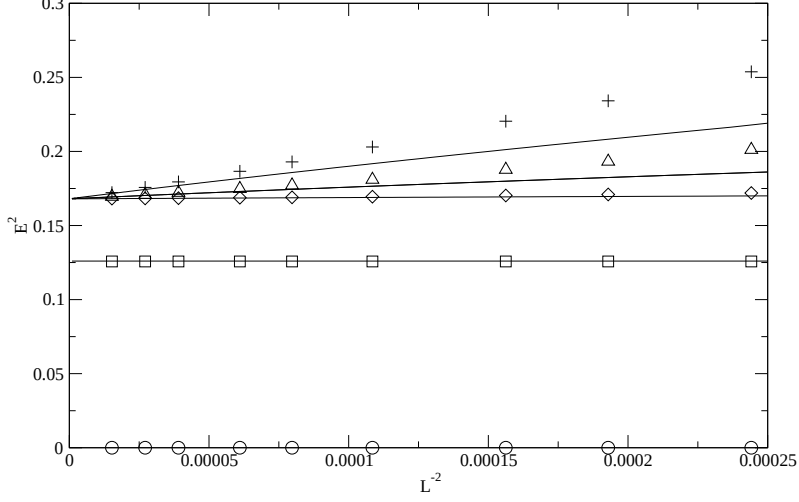


Figure 6.2: Plot of the eigenvalues E^2 of the discretised Schrödinger equation (6.42) compared with the corresponding results for the continuum with a finite box, for $\lambda = 1/16$, $m^2 = 0.084$. Plotted are the Goldstone mode (circles), the bound state (squares) and the first three scattering states (diamonds, triangles, crosses). There is a significant finite-size behaviour at this choice of m^2 , which will be worsened by radiative corrections.

The eigenvalues are compared with the continuum result, Eq. (6.13), in Figure 6.2 for $m^2 = 0.084$, $\lambda = 1/16$. These cannot be directly compared with the Monte Carlo results as the mass will pick up radiative corrections, but serve to give a qualitative description of the discretisation effects.

6.4.2 Monte Carlo simulations

Our Monte Carlo simulation uses a standard Metropolis algorithm (discussed in Section 5.1), with acceptance rates at around 70%. A hybrid Monte Carlo algorithm was tried but not used for the results presented here, as it did not deliver a significant overall improvement in performance. Generally, the space between measurements was kept longer than the autocorrelation time for the observable of interest. For the Lüscher-Wolff eigenvectors, it is impossible to determine the autocorrelation time but it was assumed to be far longer than that for the two-point function results.

Results for the kink mass

As a benchmark, we first computed the kink mass using the conventional twist method (see Section 6.2) for many different values of m^2 along the line $\lambda = 1/16$ in parameter space. The spatial average of ϕ^2 was measured for antiperiodic and periodic spatial boundary conditions, so that the mass could be calculated from Eq. (6.20). At least 2×10^5 measurements were carried out for each value of m^2 , separated by 50 update sweeps. Using the techniques set out in Section 5.2.2, the integrated autocorrelation time for ϕ^2 [102],

$$\tau_{\text{int},\phi^2} = \frac{1}{2} \sum_{\tau} \frac{\langle \phi_n^2 \phi_{n+\tau}^2 \rangle - \langle \phi_n^2 \rangle \langle \phi_{n+\tau}^2 \rangle}{\langle \phi^4 \rangle - \langle \phi^2 \rangle^2}, \quad (6.43)$$

was then estimated and used to find the number of independent measurements available for both the periodic and antiperiodic cases. The measurements were then binned appropriately. These ϕ^2 measurements were then used to calculate

$$f_1 = -\frac{1}{T} \ln \left\langle e^{-\frac{1}{2}(m_2^2 - m_1^2) \sum_x \phi^2} \right\rangle_{m_1^2}, \quad (6.44)$$

$$f_2 = \frac{1}{T} \ln \left\langle e^{-\frac{1}{2}(m_1^2 - m_2^2) \sum_x \phi^2} \right\rangle_{m_2^2} \quad (6.45)$$

in both the kink and trivial sectors. By analogy with the resampling technique of Ferrenberg and Swendsen, the measurement spacing has been made small enough that f_1 and f_2 agree, within errors, in each sector. The final errors in the kink mass derivative were estimated by applying the bootstrap method. The kink mass is then obtained by using these data to calculate

$$\Delta F(m_2^2) - \Delta F(m_1^2) = \frac{1}{2}(f_{1,\text{tw}} + f_{2,\text{tw}} - f_{1,0} - f_{2,0}) \quad (6.46)$$

where ‘tw’ demotes the results of simulations with antiperiodic (twisted) boundary conditions and ‘0’ those with periodic boundary conditions. The associated error is then

$$\Delta [\Delta F(m_2^2) - \Delta F(m_1^2)]^2 = \frac{1}{4} [\Delta f_{1,\text{tw}}^2 + \Delta f_{2,\text{tw}}^2 + \Delta f_{1,0}^2 + \Delta f_{2,0}^2 + (f_{1,\text{tw}} - f_{2,\text{tw}})^2 + (f_{1,0} - f_{2,0})^2]. \quad (6.47)$$

These expressions can then be used to find the free energy difference from some position in parameter space where it vanishes,

$$\Delta F(m_N^2) = \sum_{n=0}^{N-1} [\Delta F(m_{n+1}^2) - \Delta F(m_n^2)], \quad (6.48)$$

and hence the kink mass can be estimated.

Standard error propagation techniques can then be used to calculate the error in $M(m^2)$.

Our new method, outlined in Section 6.3.2, can be used to calculate the mass at *any* point without depending on measurements at any other. We calculate the correlator Eq. (6.25) on the lattice,

$$C(t_1 - t_2; k) = \left\langle \sum_{x_1, x_2} e^{ik(x_1 - x_2)} \phi(x_1, t_1) \phi(x_2, t_2) \right\rangle; \quad k = \frac{(2n+1)\pi}{L} \quad (6.49)$$

and fit it to A_1 , A_2 , M and E in the function

$$C(t; k) = A_1 \exp\left(-\frac{k^2}{2M} \frac{t(T-t)}{T}\right) + A_2 \left(e^{-Et} + e^{-E(T-t)}\right), \quad (6.50)$$

where the first term corresponds to the contribution (6.30) from a moving kink and the second term to a free scalar particle. A fit to either a free scalar particle or Eq. (6.30) alone does not converge. The bound state of the moving kink cannot be determined by this fit, as it will be suppressed by a factor of $1/L$.

To exclude short-range behaviour, the fit is repeated excluding more and more short-distance measurements until a ‘plateau’ for the fit parameters is reached, in line with commonly accepted practice [37]. Our error estimates for the fit are obtained by performing an elaborate bootstrap: we resample our measurements of the correlator $C(t_1 - t_2; k)$, then repeat the fit to obtain a series of estimates [46].

Our results, for varying m^2 , are shown in Figure 6.4. Our results agree with [3], in that the nonperturbative Monte Carlo result lies below the semiclassical mass result². The two measurement methods are in agreement, from very close to the phase transition to beyond $M \sim a = 1$ where

²There is an error in the equivalent calculation in [24] which was previously noted in [3].

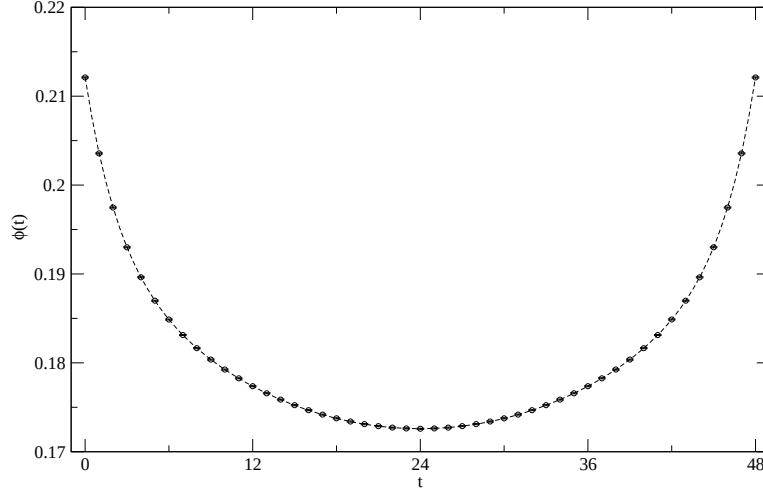


Figure 6.3: Example Monte Carlo correlator data and fit for $T = 48$, $m^2 = 0.1$, $\lambda = 1/16$ with $k = 3\pi/48$. Three points at each end are excluded from the fit.

the treatment of the kink as a semiclassical particle might be expected to break down. The same number of measurements were made for each parameter choice in both methods. This means that the overall number of measurements needed for any given point is greatly reduced by studying the two-point function, as the errors are comparable in the two cases.

In Table 6.1 we show the relative contributions of ‘kink scattering’ and ‘bulk’ behaviour to Eq. (6.49) for a value of m^2 deep in the broken phase, and a sample plot of the corresponding data is given in Figure 6.3.

Results for the particle spectrum in the presence of a kink

We measured the operators in Eq. (6.31) for separations $\Delta x = 0, 1, \dots, L/2 - 1$. An important requirement is that these operators are linearly independent; to ensure this we only use the first $L/2$ operators [61]. This is a similar imposition in position space to that of Lüscher and Wolff in momentum space for their original paper [94]. Our next step was to solve the generalised eigenvalue problem of Eq. (6.22) to give the energy spectrum.

To find the maximum time separation t at which these measurements can be taken, we used the ‘self-adjusting exponential fit’ of Göckeler et al. [61], which compares sorting by largest eigenvalue at successive times $(t, t+1)$ to

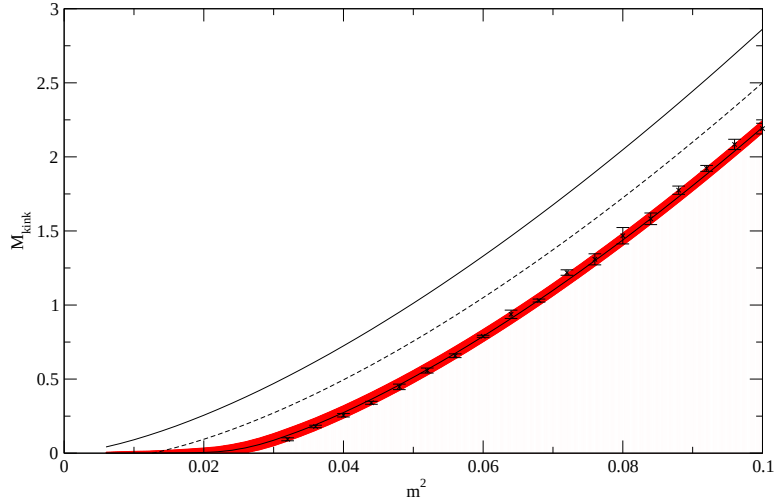


Figure 6.4: Comparison of the kink mass measurements from a twist (Section 6.2; shaded region with line at centre) and from the scattering method (Section 6.3.2; crosses). The classical result of Eq. (6.5) as well as the perturbative result Eq. (6.15) are also shown as solid and dotted lines respectively. Both types of measurement were carried out for $L = 48$; volumes $L = 32$ and $L = 40$ show finite-size effects that are similar to the magnitude of the bootstrapped errors. For the scattering measurements the errors increase when $M > 1$, but the technique is still valid.

$k = \pi/L$				
L	Kink weight A_1	Bulk weight A_2	E	M
32	2.83875 ± 0.00095	0.02293 ± 0.00081	0.38382 ± 0.01332	2.22514 ± 0.05441
40	3.02296 ± 0.00152	0.01885 ± 0.00077	0.39537 ± 0.05527	2.29455 ± 0.10858
48	3.13151 ± 0.00047	0.01743 ± 0.00019	0.41412 ± 0.00800	2.19456 ± 0.03601
$k = 3\pi/L$				
32	0.09402 ± 0.00041	0.03040 ± 0.00052	0.44331 ± 0.01196	2.04267 ± 0.07687
40	0.14710 ± 0.00043	0.02405 ± 0.00028	0.42003 ± 0.00768	2.13589 ± 0.07250
48	0.19189 ± 0.00044	0.02016 ± 0.00015	0.41473 ± 0.00602	2.18788 ± 0.04752

Table 6.1: Contributions to the correlator Eq. (6.49) from ‘kink scattering’ and ‘bulk’ behaviour for $m^2 = 0.1$ and $\lambda = 1/16$ on a $L \times L$ lattice. The errors quoted here are from a bootstrapping method. At higher momenta the kink contribution becomes smaller, relative to the bulk contribution. However, as the lattice size is increased the kink contribution increases. The kink mass remains within the error shown in Figure 6.4 for all measurements at $k = \pi/L$.

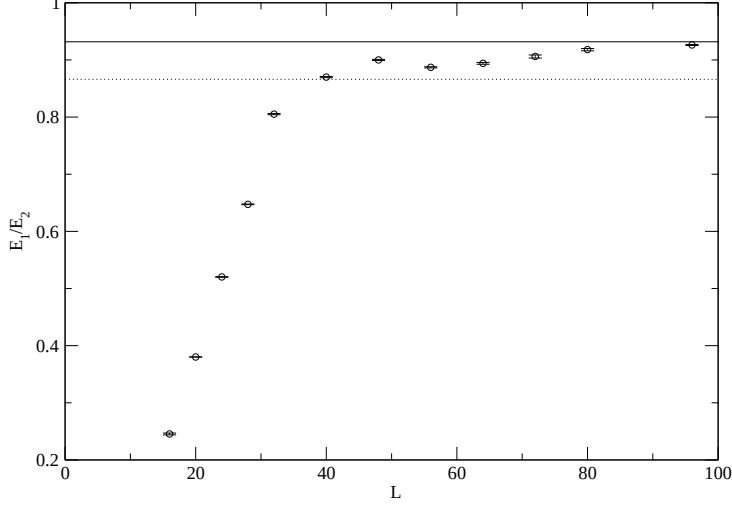


Figure 6.5: Plot of the ratio of the first to the second energy eigenvalue against lattice size, for $\lambda = 1/16$, $m^2 = 0.084$. The classical continuum result m_{bs}/m_ϕ is shown (dotted line), as well as the estimated continuum result obtained by the intercepts of Figure 6.6 (solid line). The results here are at $t = 3$.

sorting by magnitude of the scalar product of eigenvectors. The two sorting procedures no longer agree at a time t where the data are too noisy to be reliable. Another check on the extent of the noise present is the asymmetry of $C_{\Delta x, \Delta y}$. The noise in the data readily becomes apparent when fits or wavefunction reconstruction are attempted but these procedures serve as valuable checks.

In order to verify the presence of a bound, localised state in the theory, simulations were carried out on lattices of spatial size L and time size $3L$ at various lattice sizes, to see if the squeezing of the kink and the bound state could be observed. In these simulations, $\lambda = 1/16$ was used, with $m^2 = 0.084$ and $m^2 = 0.504$. These parameters have been chosen so that λ/m^2 is slightly less than unity while $1/m$ is large enough to see the squeezing of the kink at smaller lattice sizes. This squeezing effect is seen in the ratio of the bound state energy to that of the first scattering state, plotted in Figure 6.5.

The finite-size effects and the phase shift due to the kink can be seen when we attempt to extrapolate to the continuum limit (Figures 6.6 and

6.7). These should be contrasted with the Schrödinger results of Figure 6.2.

For both plots, the lowest energy level is fit to a constant since it should not have any volume dependence. For the other excitations we can include the finite-size effects. From Eq. (6.32), this motivates a fit to c_1 and c_2 in

$$E^2 = m^2 + \frac{(2n+1)^2\pi^2}{L^2} + c_1 \frac{1}{L^4} + c_2 \frac{1}{L^6} \quad (6.51)$$

for Figure 6.6. The value of m^2 is obtained from simulations with periodic boundary conditions. The data in Figure 6.7 are, however, too noisy to permit the same treatment. Instead we show the asymptotic behaviour given by the first two terms.

Eigenvectors and wavefunctions

In addition to the finite-size behaviour, further evidence for the bound state is given by the shape of the eigenvectors. In Figures 6.8 and 6.9, the eigenvectors of the correlation matrix are given for the first four energy levels at $L = 64$ (the error bars are estimates based on a bootstrap of the eigenvectors for resampled sets of measurements).

Following the method given in Section 6.3.3, these eigenvectors can be used to reconstruct the original wavefunctions. First, we estimate the renormalised mass by fitting the zero-mode energies in the periodic sector to a constant. This renormalised mass is then used in the classical gradient flow method of Eq. (6.41) to estimate the background kink.

Approximate errors are recalculated using the bootstrap method; interestingly, the errors are much smaller than those for the corresponding eigenvector. The results of the reconstruction are shown in Figures 6.8 and 6.9. In Figure 6.8 the kink is slightly wider than the lattice spatial size, and hence the bound state is ‘squeezed’.

6.5 Summary

We have shown that correlation functions in the presence of a kink provide detailed information about the kink itself: its mass and its excitation spectrum, along with the approximate wavefunctions. One can measure these correlation functions using standard Monte Carlo techniques, thereby

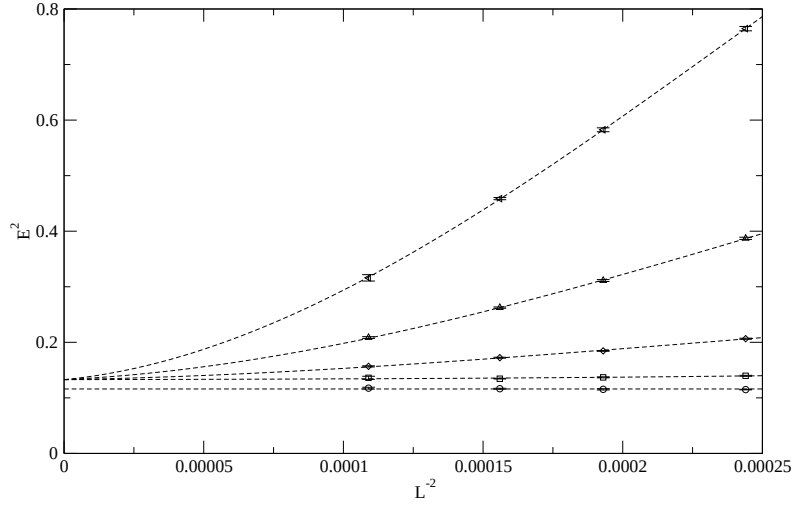


Figure 6.6: Plot of the first five energy levels given by the diagonalisation of (6.21) for the operators (6.31), with $\lambda = 1/16$, $m^2 = 0.084$. This was done at relatively short distance ($t = 2$). For the scattering states, the quality of the data here has allowed a constrained fit with two orders of discretisation effects (6.51).

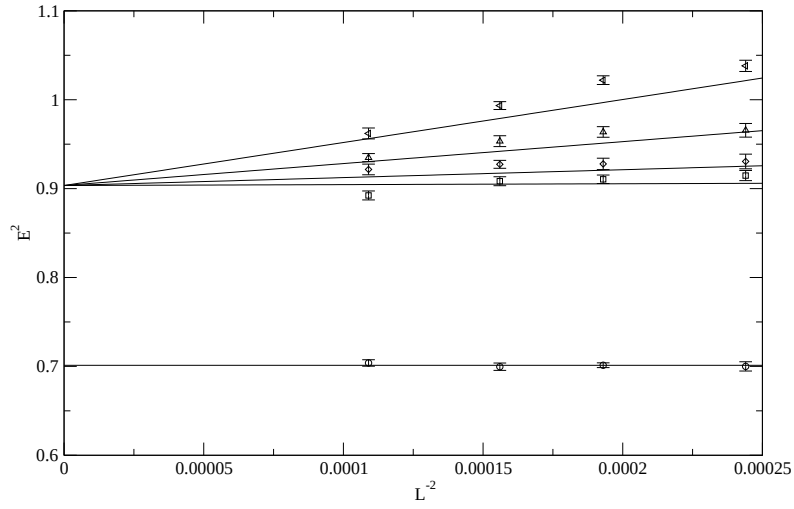


Figure 6.7: As Figure 6.6 but with $\lambda = 1/16$, $m^2 = 0.504$. Here the lines are not fits, but show the asymptotic free-particle behaviour $E^2 = m^2 + (2n + 1)^2\pi^2/L^2$.

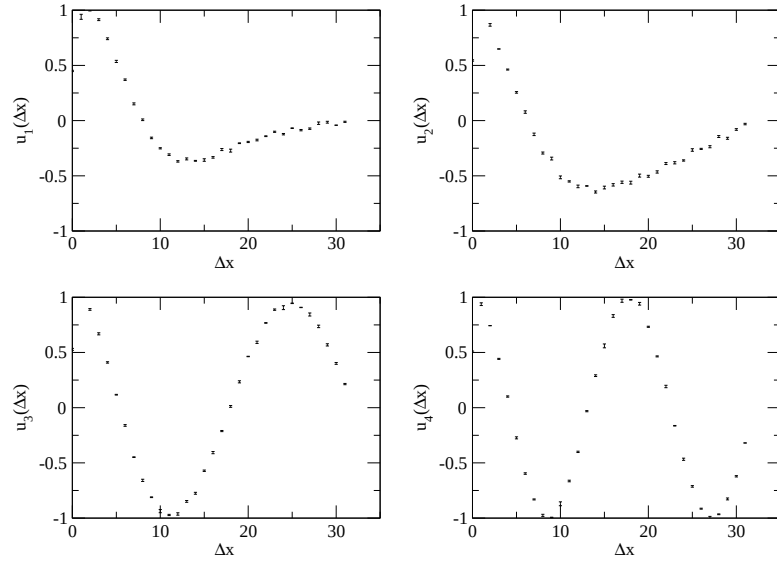


Figure 6.8: Plot of four lowest-lying eigenvectors for $L = 64$, $m^2 = 0.084$.

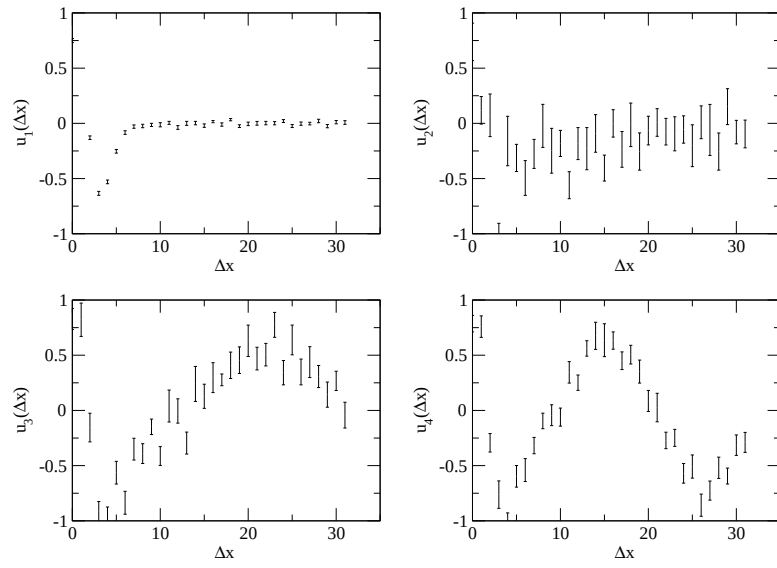


Figure 6.9: Plot of four lowest-lying eigenvectors for $L = 64$, $m^2 = 0.504$.

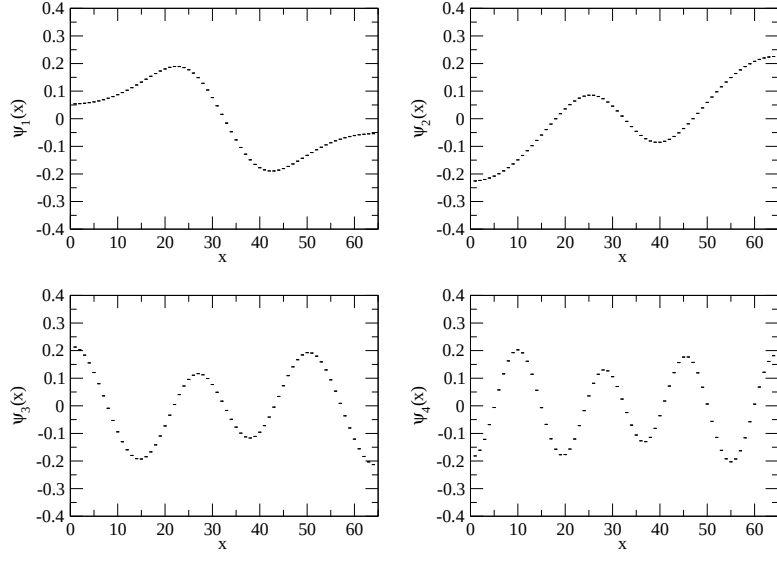


Figure 6.10: Plot of four lowest-lying wavefunctions for $L = 64$, $m^2 = 0.084$.

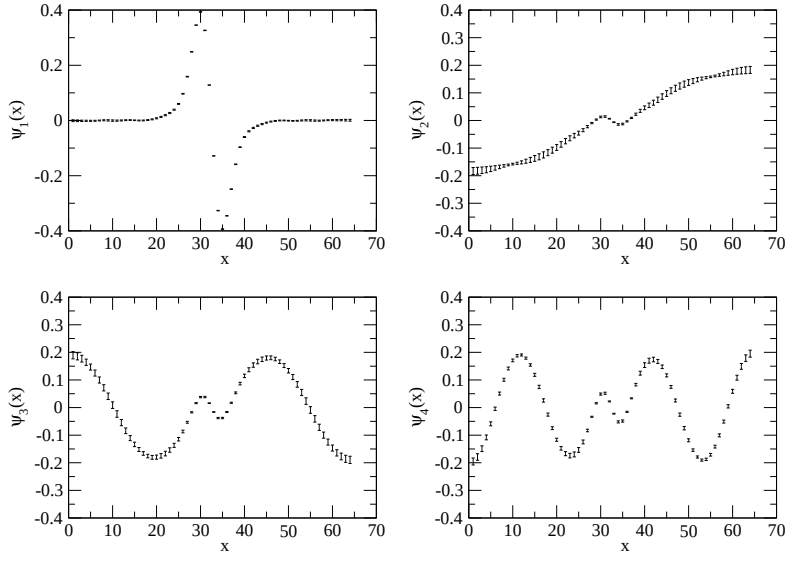


Figure 6.11: Plot of four lowest-lying wavefunctions for $L = 64$, $m^2 = 0.504$.

calculating its properties in a fully non-perturbative way in quantum field theory.

Quantum kink masses have been calculated previously in several different ways: at one-loop level in perturbation theory (see Chapter 3), and non-perturbatively using creation operators or by calculating the excess free energy of the kink across the two topological sectors (for example in Ref. [24]). Our method, in which the mass is obtained from the kinetic energy of a kink with a known momentum, is closer in spirit to the way other masses are calculated in Monte Carlo simulations, and potential errors should be better controlled.

Calculations of kink excitations have so far been restricted to the linear level, and it is quite likely that in many cases the interactions will modify even qualitative features of the spectrum, such as the number of bound states. It is therefore important to have a way of measuring the spectrum non-perturbatively. As a side product, we obtain approximate quantum wave functions of the energy eigenstates, which are only valid at weak coupling but which nevertheless help us to identify the states.

We demonstrated our methods by carrying out Monte Carlo simulations at weak coupling in the $1+1$ -dimensional $\lambda\phi^4$ theory. The results show that the mass and the excitations can be determined in practice, with relatively small errors. It will be interesting to extend these simulations to the critical region, and to see explicitly how the behaviour changes when critical phenomena become important and expectations based on linear theory become invalid. This is the focus of the calculation presented in the next chapter.

7 Soliton form factors from lattice simulations

This chapter is substantially based on work in Ref. [125], carried out with my supervisor Arttu Rajantie. Additional explanatory material and discussion, placing this work in the context of the thesis, has been added. There are also corrections to typographical errors in the equations of the paper.

Having successfully demonstrated in the previous chapter that we are able to study properties of the kink through the use of correlation functions in the topologically nontrivial sector, here we proceed one stage further and consider the consequences of studying the same model at strong coupling. The end result is a powerful test of universality: the form factor for the interaction between a scalar particle and a kink in the $\lambda\phi^4$ model is exactly the same as that in the Ising model, obtained using techniques from integrable systems.

7.1 Introduction

As seen in Chapter 3 one can, in principle, use perturbation theory to calculate ‘semiclassical’ quantum corrections to classical quantities associated with topological solitons. However, this only works when the quantum effects are small and in practice can only be used for very simple models such as the $\lambda\phi^4$ kink. A fully quantum mechanical analysis requires not only a new calculational method but also a different set of observables; the simplest classical observables do not have well-defined quantum mechanical counterparts.

In this chapter we investigate one such observable, the soliton form factor. The form factor is a fully non-perturbative quantum observable which does not rely on any semiclassical concepts, and it can be defined for any soliton in an analogous way. Form factors are used in many areas of physics to

characterise properties of quantum objects, from atomic [14] and nuclear physics [79] to integrable systems [138]. The soliton form factor describes the scattering of a particle with a soliton; it can be loosely interpreted as (the Fourier transform of) the soliton profile in the quantum theory. It is therefore the most natural quantum observable beyond the soliton mass, and it carries a large amount of non-trivial information about the soliton and its interactions. By studying the form factor, one can therefore move away completely from semiclassical ideas of soliton shape to work with fully non-perturbative results for excitations and interactions.

Choosing a concrete example with both nontrivial critical behaviour and well-understood semiclassical limits, we shall focus on the kink form factor [63, 78, 104, 105, 103] in 1+1-dimensional field theory. In the previous chapter, we studied semiclassical aspects of kinks with lattice Monte Carlo simulations by measuring the field correlation function in the presence of a kink. Here we show how that the same approach can be further developed to calculate the kink form factor in a fully non-perturbative way. We demonstrate this by carrying out simulations near the critical point, where we find excellent agreement with exact results from the two-dimensional Ising model, as predicted by universality arguments. This approach can be generalised to solitons in other theories.

7.2 Model

Let us consider a theory with a real scalar field $\phi(t, x)$ and kinks in 1+1 dimensions. Our discussion will be valid for any such theory, but as a concrete example, we use the $\lambda\phi^4$ model with the usual Lagrangian of Eqs. (6.1-6.2)

$$\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) + \frac{m^2}{2}\phi^2 - \frac{\lambda}{4!}\phi^4 - \frac{3}{2}\frac{m^4}{\lambda}. \quad (7.1)$$

We assume that the system is in a state with one kink. Classically, this simply corresponds to the exact kink solution seen in Eq. (2.17), namely

$$\phi_{\text{kink}}(x) = v \tanh(mx/\sqrt{2}) \quad (7.2)$$

where $v = m\sqrt{6/\lambda}$.

In the quantum theory, the same can be achieved by imposing twisted

antiperiodic boundary conditions in the spatial direction [67]; we already used this in the previous chapter when studying the kink mass. In fact, this only restricts the number of kinks to odd values, but states with more than one kink are exponentially suppressed in the infinite volume limit. Note that this way of preparing the system preserves translation invariance and is fully non-perturbative as it makes no reference to any classical background configuration.

The ground state $|0\rangle$ of this one-kink sector of the theory corresponds to a kink in a momentum eigenstate with zero momentum, and its energy E_0 is therefore simply the kink mass M . This state is therefore translation invariant. Above this, the spectrum consists of moving kink states $|k\rangle$ with momentum k and energy $E_k = \sqrt{k^2 + M^2}$, up to the energy E_{exc} of the first excited state of the kink. Above $M + m$, there are also states with one or more free scalar particles.

We want to calculate the kink form factor $f(k, k')$, which is defined as the matrix element

$$f(k, k') = \frac{1}{v} \langle k' | \hat{\phi}(0) | k \rangle, \quad (7.3)$$

where we have scaled it by the vacuum expectation value v to make it independent of the field normalisation, and the momentum states $|k\rangle$ have the Lorentz invariant normalisation

$$\langle k' | k \rangle = 2\pi \delta(k - k') E_k. \quad (7.4)$$

Lorentz invariance of the theory implies that, when expressed in terms of rapidities $\theta_k = \text{arcsinh } k/M$, the form factor is a function of the rapidity difference only [78], $f(k, k') = f(\theta_k - \theta_{k'})$.

Semiclassically, the kink form factor is given by the Fourier transform of the static kink solution [63, 104],

$$f_{\text{cl}}(\theta) = \frac{4}{3} i \pi v^2 \frac{1}{\sinh \frac{2}{3} \pi v^2 \theta}. \quad (7.5)$$

This can be seen by taking matrix elements of both sides of the Heisenberg equation of motion for the field. The Fourier transform is between position and rapidity space, and so has a slightly unusual normalisation to ensure

Lorentz invariance:

$$f(\theta) = M \int dx e^{iM\theta x} f(x) \quad (7.6)$$

$$f(x) = \int \frac{d\theta}{2\pi} e^{-iM\theta x} f(\theta). \quad (7.7)$$

In other words, even in the quantum theory the form factor can be thought of as the effective kink profile, to leading order. However, this interpretation should not be taken literally because, as always, there are many quantum observables that have the same semiclassical limit. The semiclassical approximation is valid at weak coupling. In our model Eq. (7.1), the dimensionless coupling is $\lambda/m^2 = 6/v^2$, thus weak coupling implies a large vacuum expectation value.

What makes the theory of Eq. (7.1) a particularly useful test bed is that the form factor is also known exactly at strong coupling, by which we mean near the critical point $m^2 \approx m_c^2$ in the quantum theory.

The theory is in the same universality class as the two-dimensional Ising model, and near the critical point the form factor should approach the exact Ising model result [7, 159],

$$f_{\text{Ising}}(\theta) = i \coth \frac{\theta}{2}. \quad (7.8)$$

Matrix elements like Eq. (7.3) cannot be computed directly using Monte Carlo simulations. Instead, the basic observable is the field correlation function, which we consider in the ground state $|0\rangle$ of the one-kink sector. We calculate it in momentum space, taking the Fourier transform in space but not in time, and write a spectral expansion in terms of energy eigenstates $|\alpha\rangle$ with energies E_α ,

$$\langle \phi(0, k) \phi(t, q) \rangle = \sum_{\alpha} \frac{\langle 0 | \hat{\phi}(k) | \alpha \rangle \langle \alpha | \hat{\phi}(q) | 0 \rangle}{\langle 0 | 0 \rangle} e^{it(E_\alpha - E_0)}. \quad (7.9)$$

Lattice Monte Carlo simulations are carried out in Euclidean space, which is obtained by carrying out a Wick rotation $t \rightarrow it$. This does not affect the coefficients of the spectral expansion, but the exponentials become real and

the result is that previously seen as Eq. (4.23),

$$\langle \phi(0, k) \phi(t, q) \rangle = \sum_{\alpha} \frac{\langle 0 | \hat{\phi}(k) | \alpha \rangle \langle \alpha | \hat{\phi}(q) | 0 \rangle}{\langle 0 | 0 \rangle} e^{-t(E_{\alpha} - E_0)}. \quad (7.10)$$

At long enough time separation,

$$t \gg \frac{1}{E_{\text{exc}} - E_0}, \quad (7.11)$$

the dominant contribution comes from the single-particle moving kink states $|k\rangle$. For them, the coefficient of the expansion is essentially the form factor, because

$$\langle k' | \hat{\phi}(q) | k \rangle = v f(k, k') 2\pi \delta(k - q - k'). \quad (7.12)$$

The momentum conservation delta function restricts the expansion to only states with overall momentum k , and therefore we have

$$\begin{aligned} \langle \phi(0, k) \phi(t, q) \rangle &= \frac{2\pi \delta(k + q)}{L} \frac{v^2 |f(k, 0)|^2}{E_k E_0} e^{-t(\sqrt{k^2 + M^2} - M)} \\ &+ O\left(e^{-t(E_{\text{exc}} - M)}\right), \end{aligned} \quad (7.13)$$

where L is the spatial length of the system, and we have used $\langle 0 | 0 \rangle = L E_0$ as implied by our normalisation.

Furthermore, the Euclidean spacetime is necessarily finite in actual Monte Carlo simulations. We assume periodic boundary conditions in the time direction, and denote the length of the system by T . In the periodic Euclidean time, the field correlator is given by Eq. (4.22)

$$\langle \phi(0, k) \phi(t, q) \rangle = \frac{\text{Tr} \hat{U}(T - t) \hat{\phi}(q) \hat{U}(t) \hat{\phi}(k)}{\text{Tr} \hat{U}(T)}, \quad (7.14)$$

where $\hat{U}(t) = \exp(-\hat{H}t)$ is the Euclidean time evolution operator. As in Eq. (7.10), at long enough time separations the only contribution comes from single-particle kink momentum eigenstates $|k\rangle$, so we can approximate the trace in Eq. (7.14) by an integral over them,

$$\langle \phi(0, k) \phi(t, q) \rangle = \frac{\int \frac{dk'}{2\pi E_{k'}} \langle k' | \hat{U}(T - t) \hat{\phi}(q) \hat{U}(t) \hat{\phi}(k) | k' \rangle}{\int \frac{dk'}{2\pi E_{k'}} \langle k' | \hat{U}(T) | k' \rangle}. \quad (7.15)$$

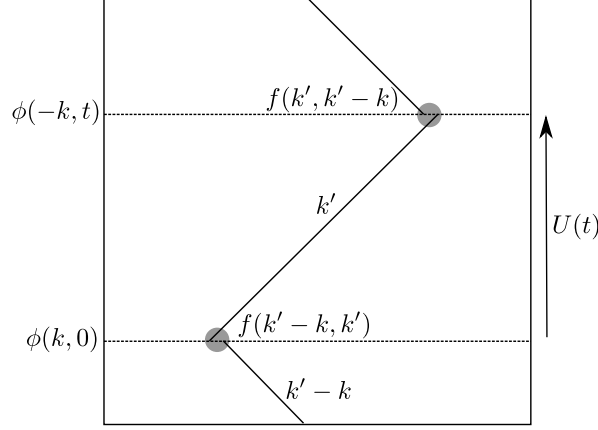


Figure 7.1: Illustration corresponding to Eq. (7.18). The kink is constrained by periodic boundary conditions in the Euclidean time direction, so the worldline must match up at either end of the lattice. The defect is not point-like, and has a form factor which is represented here by the interaction between the scalar and the defect having a finite size.

Using

$$\langle k' | \hat{U}(t) | k \rangle = 2\pi \delta(k - k') E_k e^{-E_k t}, \quad (7.16)$$

we can write the denominator as

$$\int \frac{dk'}{2\pi E_{k'}} \langle k' | \hat{U}(T) | k' \rangle = L \int \frac{dk'}{2\pi} e^{-E_{k'} T}. \quad (7.17)$$

Inserting complete sets of momentum eigenstates, the numerator becomes

$$\begin{aligned} & \int \frac{dk'}{2\pi E_{k'}} \langle k' | \hat{U}(T-t) \hat{\phi}(q) \hat{U}(t) \hat{\phi}(k) | k' \rangle \\ &= 2\pi \delta(q+k) \int \frac{dk'}{2\pi} \frac{v^2 |f(k'-k, k')|^2}{E_{k'-k} E_{k'}} e^{-E_{k'}(T-t) - E_{k'-k} t}. \end{aligned} \quad (7.18)$$

As illustrated in Figure 7.1, this integral has a simple geometrical interpretation: The kink travels from time 0 to time t at momentum $k' - k$, where it interacts with a ϕ particle. This changes its momentum to k' , with which it moves forward in time through the periodic boundary back to time 0. In contrast to Figure 6.1, however, the interaction between kink and scalar particle is no longer pointlike; it carries a form factor f .

To calculate the integrals (7.17) and (7.18), we use the saddle point approximation. The saddle point k_0 for Eq. (7.18) is found by minimising the action

$$S(k') = E_{k'}(T - t) + E_{k'-k}t - MT \quad (7.19)$$

for given t . By approximating the integral by a Gaussian around the saddle point, we obtain

$$\langle \phi(0, k) \phi(t, q) \rangle = \frac{2\pi\delta(k + q)}{L} \sqrt{\frac{T}{M}} \frac{v^2 |f(k_0, k_0 - k)|^2}{E_{k_0-k} E_{k_0} \sqrt{S''(k_0)}} e^{-S(k_0)}. \quad (7.20)$$

This approximation is only valid when the action is sufficiently peaked and well approximated by a Gaussian. The latter assertion requires

$$S''(k_0)^2 \gg S^{(4)}(k_0). \quad (7.21)$$

This implicitly imposes a lower limit for the system size T in the time direction, so for higher k we need to use larger lattices. As usual, the lattice size also has to be larger than any inverse mass, including the kink mass M .

Finally, we note that because ϕ is real and the kink has odd parity, the form factor is odd and purely imaginary. Therefore we can use Eq. (7.20) to determine it from the field correlator, up to a sign. For given k and t , we obtain the saddle point k_0 by minimising Eq. (7.19), and the form factor for rapidity difference θ is given by

$$\begin{aligned} f(\theta) &= f(k_0, k_0 - k) \\ &= \pm i \frac{\sqrt{\langle \phi(0, k) \phi(t, -k) \rangle}}{v} \left(\frac{M}{T} \right)^{1/4} \sqrt{E_{k_0-k} E_{k_0}} (S''(k_0))^{1/4} e^{S(k_0)} \end{aligned} \quad (7.22)$$

where

$$\theta = \operatorname{arcsinh} \frac{k_0}{2M} - \operatorname{arcsinh} \frac{k_0 - k}{2M}. \quad (7.23)$$

While Eq. (7.22) is an approximation, it becomes exact for sufficiently large T as discussed above; one must also satisfy Eq. (7.11) by excluding small t .

7.3 Results

We tested this result by calculating the form factor near the critical point using lattice Monte Carlo simulations.

Recalling Eq. (6.39), the Euclidean lattice action for the theory (7.1) is given in lattice units by

$$S = \sum_{\mathbf{x}} \left[- \sum_{\mu=1}^2 \phi(\mathbf{x}) \phi(\mathbf{x} + \hat{\mu}) + \left(2 - \frac{m^2}{2} \right) \phi(\mathbf{x})^2 + \frac{\lambda}{4!} \phi(\mathbf{x})^4 \right] \quad (7.24)$$

with $\lambda = 0.6$. Square lattice sizes of $L = T \in \{125, 250, 375\}$ were used. A kink is created by imposing antiperiodic boundary conditions in the space direction, $\phi(x + L, t) = -\phi(x, t)$. This also leads to discretisation of momentum, $k = (2n + 1)\pi/L$.

We measured the momentum space unequal-time field correlator at various time separations and then used Eq. (7.22) to calculate the form factor for various rapidities. At the strong couplings used here, the correlator measurements are reliable even at very long distance thanks to the hybrid Monte Carlo algorithm (discussed in Section 5.1.1) which was helpful in fighting critical slowing down and thermalising long-distance modes efficiently. In principle, Eq. (7.22) gives the form factor for a range of θ from a single choice of parameters $\{k, L, m^2\}$ because the same simulation gives the correlator for all values of the time separation t . However, these values are strongly correlated; we report only one data point per combination with a quoted error obtained from a bootstrap resampling of all measurements. This technique was discussed in greater detail in Section 5.2.5.

Given Eq. (7.11), the time separation t has to be long enough that excited states and two-particle states are suppressed sufficiently. This happens when $t \gtrsim 1/2M$. However, at greater distances statistical noise starts to grow. Therefore, we select the value of t with the smallest statistical error within the permitted range.

In addition to the field correlator, Eq. (7.22) also involves the vacuum expectation value v of ϕ , and the kink mass M . We measured v using simulations with periodic boundary conditions. We take the ensemble average $v = \langle |\sum_{x \in V} \phi(x)| \rangle$ of the average field's absolute value.

To obtain the kink mass M , we again used Eq. (7.15) and the saddle point

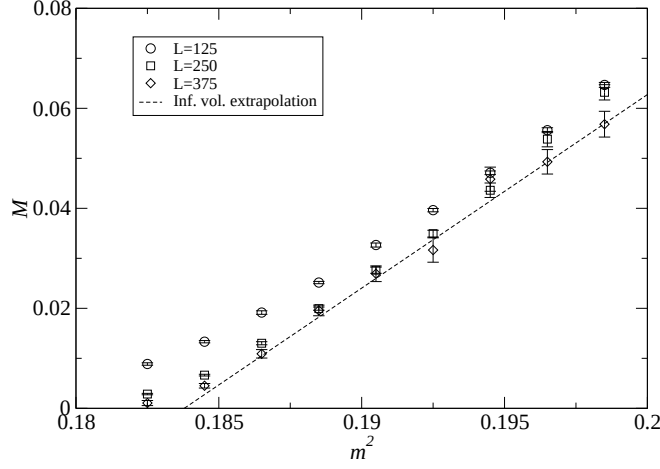


Figure 7.2: The kink mass M as a function of m^2 in different volumes. The data agree with the known results for the Ising universality class [1]: extrapolating to the infinite-volume limit, the dependence on m^2 is linear.

approximation, but this time taking the lowest available momentum, $k = \pi/L$, leaving the higher momentum measurements as independent datasets for study of the form factor. Then, as long as $k \ll M$, Eq. (7.19) simplifies and we find the saddle point $k_0 = kt/T$ for arbitrary t . We can, therefore, apply the saddle point approximation analytically, and we find [124]

$$\langle \phi(0, k) \phi(t, q) \rangle \propto e^{-\sqrt{M^2 + k_0^2} t - \sqrt{M^2 + (k - k_0)^2} (T - t) + MT}. \quad (7.25)$$

This reduces to Eq. (6.30) in the nonrelativistic limit.

We then fit the $k = \pi/L$ correlator data to Eq. (7.25) to obtain the mass M with a bootstrap error. The results of this fitting are shown in Figure 7.2. Alternatively, the mass could also be calculated from the free energy difference between the kink and vacuum sectors [67].

This way, we have measured all the quantities that appear in Eq. (7.22). We can calculate the form factor $f(\theta)$ at a wide range of rapidities for different momenta and different values of m^2 . Finally, we have checked the consistency of the saddle point approximation leading to Eq. (7.20) when

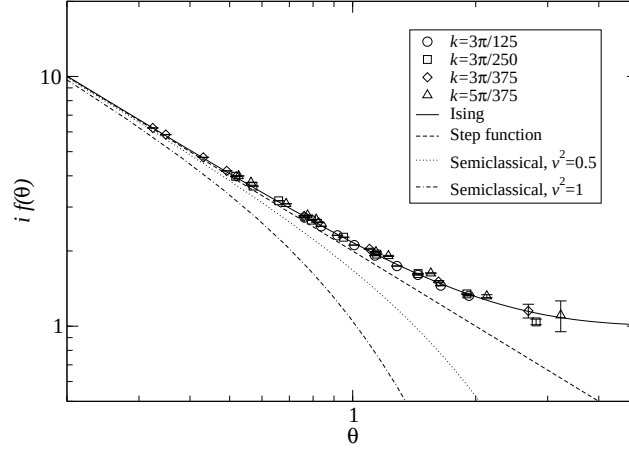


Figure 7.3: The kink form factor as a function of the rapidity difference. Measurements are shown for several lattice sizes at various momenta, and the form factors for the Ising model and for a semiclassical kink are also shown.

Eq. (7.21) is satisfied.

The results in the critical regime are shown in Figure 7.3, together with the exact Ising model result Eq. (7.8) for comparison. The agreement is very good.

7.4 Summary

We have, therefore, demonstrated that we can calculate the kink form factor reliably even at strong coupling where perturbative approaches fail. Unlike the Ising model, the scalar field theory of Eq. (7.1) in which we carried out the calculation is not exactly solvable, and we made no use of any special features of the theory. Therefore we expect that the same method will work equally well in other theories.

It is this final assertion that we seek to test in the next chapter, by looking at the mass and form factors of a rather more complicated object – the 't Hooft-Polyakov monopole – using the techniques presented and validated in this and the previous chapter.

8 Form factors of a 't Hooft-Polyakov Monopole

The material in this chapter is developed from research conducted in collaboration with my supervisor that has recently made available as an e-print as Ref. [126]. This work has been submitted to a journal for review. Some additional explanatory material and equations have been included, but the results and technique are unchanged.

8.1 Introduction

We saw in Chapter 1 that theorising about the origins of magnetism has been going on for hundreds of years. The existence of just one monopole is enough to explain why magnetic charge is quantised [40]. They are also a general prediction of grand unified field theories [145, 117].

Furthermore, Chapter 3 discussed the limited progress that has been made towards studying the non-supersymmetric quantum 't Hooft-Polyakov monopole analytically; the only perturbative result is the one-loop logarithmic correction of Eq. 3.49.

In the previous two chapters, we developed or adapted techniques for the nonperturbative study of topological defects, their intrinsic properties and their excitations. In the present chapter we hope to demonstrate their ready applicability to a much more sophisticated system possessing defect solutions. We shall also identify the ways in which the addition of a gauge field makes a substantive difference to the physics.

The Lagrangian of the SU(2) Georgi-Glashow model under investigation is

$$\mathcal{L} = -\frac{1}{4}\text{Tr}F_{\mu\nu}F^{\mu\nu} + \text{Tr}[D_\mu, \Phi][D^\mu, \Phi] - m^2\text{Tr}\Phi^2 - \lambda(\text{Tr}\Phi^2)^2 \quad (8.1)$$

with the covariant derivative $D_\mu = \partial_\mu + igA_\mu$. The field Φ is in the adjoint

representation of the SU(2) gauge group and can be parameterised by the Pauli matrices as $\Phi = \phi^a \sigma^a$.

In the broken phase, which occurs classically for $m^2 < 0$ in the parameterisation chosen here, a vacuum expectation value $\text{Tr } \Phi^2 = -m^2/2\lambda = v^2$ forms, and the SU(2) symmetry is broken to U(1). In this phase, the theory has monopole solutions with an extended scalar field (see their derivation in Chapter 2, and Refs. [145, 117]).

Even in continuum, the classical profile of this monopole solution must be obtained numerically except in the BPS limit where $\lambda \rightarrow 0$. The classical mass of the monopole can be written as

$$M = \frac{4\pi m_W}{g^2} f(z), \quad (8.2)$$

where $f(z)$ is a function of the ratio $z = m_H/m_W$, $m_H = \sqrt{2}|m|$ is the Higgs mass and $m_W = g|m|/\sqrt{\lambda}$ is the mass of the charged $W^\pm$ bosons. For non-zero z , the function $f(z)$ needs to be calculated numerically or as a Taylor expansion [55, 86].

Two length scales can be associated with the quantum monopole. The first is the Compton wavelength determined by the monopole mass M ; the other is the core size of the monopole which is determined by the perturbative masses m_H and m_W . Eq. (8.2) shows that at weak coupling there is a large hierarchy between these scales, $M \gg m_W, m_H$.

8.2 Lattice implementation

In order to study the theory (8.1) using Monte Carlo simulations, we Wick rotate it to 4D Euclidean space and discretise it. Our Euclidean lattice action is

$$\begin{aligned} \mathcal{L}_E = 2 \sum_{\mu} \left[\text{Tr} \Phi(\vec{x})^2 - \text{Tr} \Phi(\vec{x}) U_{\mu}(\vec{x}) \Phi(\vec{x} + \hat{\mu}) U_{\mu}^{\dagger}(\vec{x}) \right] \\ + \frac{2}{g^2} \sum_{\mu < \nu} [2 - \text{Tr } U_{\mu\nu}(\vec{x})] + m^2 \text{Tr } \Phi^2 + \lambda (\text{Tr } \Phi^2)^2 \end{aligned} \quad (8.3)$$

with link matrices parameterised as $U_{\mu} = 1 + i\sigma_a u_a$. We have set the lattice spacing to unity, and therefore are left with the electric charge g , bare mass m and quadratic coupling λ as free parameters.

In the symmetry broken phase, a residual U(1) symmetry persists. We can derive link variables u_μ corresponding to this smaller gauge group [34, 45]

$$u_\mu = \Pi_+(x)U_\mu(x)\Pi_+(x + \hat{\mu}) \quad (8.4)$$

where $\Pi_+ = \frac{1}{2}(1 + \hat{\Phi})$ and $\hat{\Phi} = \Phi\sqrt{2/\text{Tr } \Phi^2}$, giving an Abelian field strength tensor

$$\alpha_{\mu\nu} = \frac{2}{g} \arg \text{Tr } u_\mu(x)u_\nu(x + \hat{\mu})u_\mu^\dagger(x + \hat{\nu})u_\nu^\dagger(x) \quad (8.5)$$

and an expression for the lattice magnetic field,

$$B_i = \frac{1}{2}\epsilon_{ijk}\alpha_{jk}. \quad (8.6)$$

Gauss's law for a magnetic field in standard U(1) electrodynamics is $\nabla \cdot \mathbf{B} = 0$. The presence of magnetic monopoles means that the right hand side is no longer zero everywhere. Denoting the magnetic charge density ρ_M , the lattice equivalent of the magnetic Gauss's law becomes

$$\sum_{i=1}^3 [B_i(\mathbf{x} + \hat{i}) - B_i(\mathbf{x})] = \rho_M(x) = \frac{4\pi n}{g} \quad (8.7)$$

where n is an integer, which can be non-zero; magnetic charges are permitted. In the classical limit, these charges correspond to 't Hooft-Polyakov monopoles [145, 117]. Note that even on the lattice, the magnetic charge is quantised and localised in one lattice cell. This should be compared to the $\lambda\phi^4$ kink of previous chapters. There the topological charge can only be determined asymptotically, as we discussed in Chapter 2.

We simulate the theory of Eq. (8.3) on a Euclidean lattice of size¹ $L^3 \times T$. To create nonzero magnetic charge we apply twisted boundary conditions on each timeslice [34], while retaining periodic boundary conditions in the time direction. The twisted spatial boundary conditions are (see Figure 8.1)

$$\begin{aligned} \Phi(x + L\hat{i}) &= \sigma_i \Phi(x) \sigma_i \\ U(x + L\hat{i}) &= -\sigma_i U(x) \sigma_i \end{aligned} \quad (8.8)$$

¹We choose this notation to be consistent with earlier literature. Note that our T is not temperature, and even though we work in 4D Euclidean space one should not interpret it as the imaginary time formulation of finite-temperature field theory. If one were to use that interpretation, the temperature of the system would be $1/T$.

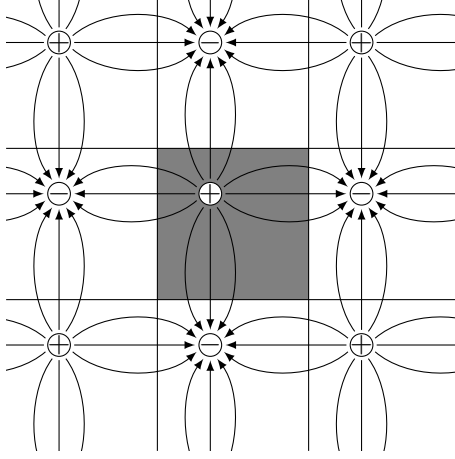


Figure 8.1: A two-dimensional spatial slice through the system with boundary conditions of Eq. (8.8). The magnetic field lines are shown, and the antiperiodicity of the magnetic field components can be deduced. The simulated box is shaded, with ‘image’ magnetic charges shown in the neighbouring boxes. It can be seen that moving from the boundary on one side of the lattice to the other requires that the magnetic field be reversed.

in the i th. direction, where σ_i is the appropriate Pauli matrix. These boundary conditions force the magnetic charge to be odd. If T is large enough then the contribution to the partition function for the simulation with these boundary conditions must come predominantly from the one-charge sector as tunnelling is heavily suppressed. Specifically, we have a partition function

$$Z_{\text{tw}} = 2Z_0 \left(Z_1 e^{-MT} + \frac{1}{3!} Z_1^3 e^{-3MT} + \dots \right), \quad (8.9)$$

where

$$Z_1 = (ML^2 T / 2\pi)^{3/2} \quad (8.10)$$

is the partition function for an isolated pointlike monopole (and, in fact, the usual partition function for a point particle at *temperature* $1/T$ – see footnote 1).

Similar arguments apply to the C-periodic boundary conditions

$$\begin{aligned}\Phi(x + L\hat{i}) &= \sigma_2 \Phi(x) \sigma_2 \\ U(x + L\hat{i}) &= -\sigma_2 U(x) \sigma_2,\end{aligned}\tag{8.11}$$

which are locally gauge equivalent to the twisted ones (8.8), but not globally. These boundary conditions permit only even magnetic charges, with the resulting partition function taking the form

$$Z_C = Z_0 + 2Z_0 \left(Z_1^2 \frac{1}{2!} e^{-2MT} + \dots \right).\tag{8.12}$$

While the Higgs field is periodic with these boundary conditions, the magnetic field – as defined by Eq. (8.6) – remains antiperiodic. By contrast, standard periodic boundary conditions only permit zero total charge since the magnetic field is also periodic.

In the continuum limit, we would expect a magnetic Coulomb’s law of the form (for a point charge)

$$\mathbf{B} = \frac{4\pi}{g} \frac{\mathbf{r}}{4\pi r^3} = \frac{1}{g} \frac{\mathbf{r}}{r^3}.\tag{8.13}$$

Later in the paper we will study the two-point function of this $\mathbf{B}$ with twisted boundary conditions. It is useful to note at this point that the effect of Eq. (8.8) is to reverse the direction of the magnetic field at the boundary and so only antiperiodic components of the Fourier transform of the magnetic field may be measured (see Figure 8.1). This is in contrast to $\text{Tr } \Phi^2$ which is manifestly periodic at the boundaries in all three spatial directions.

Simulating the system with a Euclidean time direction has two important benefits. Firstly, it prevents the monopole appearing instantonic [33]. Second, we are able to carry out measurements of the low-lying one-particle states in the quantum field theory with unequal time two-point correlators, which is the main technique used in this chapter. We can exploit the properties of the energy spectrum of the system – the quantised monopole having a lower excitation energy than even the quantised photon – and the long-distance behaviour of the magnetic monopole contribution, to obtain the monopole mass and interactions from straightforward fitting techniques.

8.3 Free energy as the response to a twist

As we discussed in Chapter 6, the conventional technique for studying magnetic monopoles and other topological defects with lattice Monte Carlo simulations has consisted of measuring their mass via their free energy.

The mass of the monopole is obtained from the difference in free energies in the two different topological sectors. This, in turn, must be obtained from the partition functions through

$$\Delta F = F_{\text{tw}} - F_{\text{C}} = -\frac{1}{T} \ln \frac{Z_{\text{tw}}}{Z_{\text{C}}}. \quad (8.14)$$

From this, we can obtain the mass using Eqs. (8.9) and (8.12), which give

$$\Delta F = MT - \ln 2 + \frac{3}{2} \ln \frac{ML^2}{2\pi T} + O(e^{-2MT}). \quad (8.15)$$

Unfortunately, we cannot measure partition functions in Monte Carlo simulations (though we can, in principle, measure the ground state energy difference using other nonperturbative techniques [69]). Instead one can integrate along a path from a point in parameter space where the free energy (and mass) of the monopole are known to vanish to the point where the mass is required. If we just differentiate Eq. (8.14) with respect to a parameter in the Lagrangian, we get

$$\Delta F = \int dg \left[\left\langle \frac{\partial S}{\partial g} \right\rangle_{\text{tw}} - \left\langle \frac{\partial S}{\partial g} \right\rangle_{\text{C}} \right]. \quad (8.16)$$

We can integrate this expression from the symmetric phase where the monopole has zero mass, through the phase transition, to our desired value of m^2 in the broken phase. Here, we use this technique as a benchmark for comparison of our correlator results. However, as in Chapter 6, we use finite differences instead of trying to integrate Eq. (8.16) directly.

The free energy of an ensemble is defined as $F = -\ln Z$, where

$$Z = \int \mathcal{D}U_i \mathcal{D}\Phi e^{-S} \quad (8.17)$$

is the partition function. The derivative of the free energy difference (8.14)

is therefore

$$\frac{\partial \Delta F}{\partial g} = \left[\left\langle \frac{\partial S}{\partial g} \right\rangle_{\text{tw}} - \left\langle \frac{\partial S}{\partial g} \right\rangle_{\text{C}} \right], \quad (8.18)$$

where the subscripts indicate expectation values calculated in the two ensembles. In our calculations, we take $g = m^2$, yielding

$$\frac{\partial \Delta F}{\partial m^2} = [\langle \text{Tr } \Phi^2 \rangle_{\text{tw}} - \langle \text{Tr } \Phi^2 \rangle_{\text{C}}]. \quad (8.19)$$

Integrating this expression from the symmetric phase where $M = 0$ through the phase transition to our desired value of m^2 will yield, in principle, the mass M . However, it is difficult to obtain reliable error estimates from this technique; it is important that we keep the error estimates under control.

In practice, one uses finite differences instead of the derivative (8.19). The free energy difference between two different values of m^2 can be written in two ways,

$$f_1 = -\ln \left\langle e^{-(m_2^2 - m_1^2) \sum_x \text{Tr } \Phi^2} \right\rangle_1 \quad (8.20)$$

and

$$f_2 = \ln \left\langle e^{-(m_1^2 - m_2^2) \sum_x \text{Tr } \Phi^2} \right\rangle_2 \quad (8.21)$$

where the expectation values are calculated at m_1^2 and m_2^2 . Having established that the two measurements f_1 and f_2 are in agreement, the change in the free energy is

$$\Delta F(m_2^2) - \Delta F(m_1^2) = \frac{1}{2} (f_1^{\text{tw}} + f_2^{\text{tw}} - f_1^{\text{cl}} - f_2^{\text{cl}}), \quad (8.22)$$

where we have chosen to average f_1 and f_2 with equal weights. The errors for f_1 and f_2 for each sector are added in quadrature and therefore we have

$$\begin{aligned} \Delta [\Delta F(m_2^2) - \Delta F(m_1^2)]^2 &= \frac{1}{4} [\Delta f_{1,\text{tw}}^2 + \Delta f_{2,\text{tw}}^2 + (f_{1,\text{tw}} - f_{2,\text{tw}})^2 \\ &\quad + \Delta f_{1,\text{C}}^2 + \Delta f_{2,\text{C}}^2 + (f_{1,\text{C}} - f_{2,\text{C}})^2] \end{aligned} \quad (8.23)$$

We know $M = 0$ in the symmetric phase, so we start summing the differences from a value of m^2 where the symmetry is not yet broken. Whereas the errors in each f for a change from m_1^2 to m_2^2 are themselves independent, there is a small nonzero covariance for two different adjacent steps. Some

care is therefore needed when summing all the errors in a mass measurement.

As a check, we should make sure that our measurements of f_1 and f_2 are concordant, since they measure the same thing. This ensures that the two ensembles at m_1^2 and m_2^2 are thermalised and at equilibrium, and the spacing is sufficiently small that the histograms of data for $\text{Tr } \Phi^2$ overlap adequately. Ferrenberg and Swendsen's work (discussed in Section 5.2.1) encourages us to see this process as the reweighting of a histogram of measurements, and their formula immediately yields

$$P_{m_2^2}(\text{Tr } \Phi^2) = \frac{P_{m_1^2}(\text{Tr } \Phi^2) e^{(m_2^2 - m_1^2) \text{Tr } \Phi^2}}{\sum_{\text{Tr } \Phi^2} P_{m_1^2}(\text{Tr } \Phi^2) e^{(m_2^2 - m_1^2) \text{Tr } \Phi^2}} \quad (8.24)$$

for the observed distribution of $\text{Tr } \Phi^2$ sampled at m_1^2 and evaluated at m_2^2 [51]; interchanging m_1^2 and m_2^2 gives the expression for measurements sampled at m_2^2 evaluated at m_1^2 . The equality $f_1 = f_2$ then follows, but the importance of this approach is the realisation that the measurements will not agree unless sufficient overlap of the histograms for $\text{Tr } \Phi^2$ at both m_1^2 and m_2^2 are available. This overlap means that the difference in the actions, $\Delta S = \sum_x (m_2^2 - m_1^2) \text{Tr } \Phi^2$, should be relatively small.

Less overlap means the inferred value of $\text{Tr } \Phi^2$ is an over (or under) estimate, being closer to the original value than required. This will make f_1 and f_2 too big, so the free energy will be overestimated. A similar overestimate will occur in both topological sectors, although $\sum_x \text{Tr } \Phi^2$ is smaller in the topologically nontrivial sector.

Because we can use this approach to accurately interpolate the free energy of the monopole at any value of m^2 , the result is plotted continuously on Figures 8.2 and 8.3. If we encounter difficulty obtaining good statistics, then this technique would be ideal to use alongside parallel tempering (replica exchange Monte Carlo), due to the necessarily small separations between values of m^2 [144]. In our case replica exchange would have been usable if the measurement spacings were slightly smaller, but would have led to substantial wait times with our computer cluster.

8.4 Two-point functions

In carrying out our lattice simulations, we follow the measurement protocol developed over the last two chapters. First we use the lowest momentum correlators to measure the monopole mass, then compare with the ‘response to a twist’ measurements used previously. In addition to the exponential long-distance behaviour of the two-point correlator giving us the energy of the excited defect state, we can also use the amplitude of the defect contribution to the correlator (as determined by a fit) to measure the form factor for various interactions.

The form factor, defined for a local operator $\hat{\mathcal{O}}$ as

$$f(\mathbf{p}_2, \mathbf{p}_1) = \langle \mathbf{p}_2 | \hat{\mathcal{O}}(0) | \mathbf{p}_1 \rangle, \quad (8.25)$$

where $|\mathbf{p}_1\rangle$ and $|\mathbf{p}_2\rangle$ are momentum eigenstates, is a useful way of studying the interaction of $\hat{\mathcal{O}}$ with the monopole. These momentum eigenstates are normalised in a Lorentz-invariant way as

$$\langle \mathbf{p}' | \mathbf{p} \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{p}' - \mathbf{p}) E_{\mathbf{p}}. \quad (8.26)$$

The form factor is also closely related to the scattering amplitude between the monopole and the particle created by operator $\mathcal{O}$.

We shall start by looking at analytical and semiclassical results for the form factor of the monopole with various quantities, then go on to generalise the results of the previous chapter to the present case. These results will allow us to relate quantities measured in lattice simulations to scalar-monopole and photon-monopole form factors.

8.4.1 Form factors: semiclassical results

In the semiclassical limit, the form factor is given by the Fourier transform of the classical profile $\mathcal{O}_{\text{cl}}(x)$ of the quantity $\mathcal{O}$ in the monopole configuration,

$$\begin{aligned} f(\mathbf{p}_2, \mathbf{p}_1) &= \langle \mathbf{p}_2 | \hat{\mathcal{O}}(0) | \mathbf{p}_1 \rangle \\ &= \sqrt{E_{\mathbf{p}_2} E_{\mathbf{p}_1}} \int d^3x e^{i(\mathbf{p}_2 - \mathbf{p}_1) \cdot \mathbf{x}} \mathcal{O}_{\text{cl}}(\mathbf{x}) \\ &\approx M \int d^3x e^{i(\mathbf{p}_2 - \mathbf{p}_1) \cdot \mathbf{x}} \mathcal{O}_{\text{cl}}(\mathbf{x}), \end{aligned} \quad (8.27)$$

where the last line is valid in the non-relativistic limit, when $|\mathbf{p}_1|, |\mathbf{p}_2| \ll M$. This agrees with the Fourier transform pair of Eqs. (7.6-7.7), where the argument was framed in terms of taking matrix elements for the Heisenberg equation of motion for the field.

In the non-relativistic limit, to which we restrict ourselves, the form factor becomes a function of the momentum difference $\mathbf{k} \equiv \mathbf{p}_2 - \mathbf{p}_1$ only as a direct consequence of Galilean invariance, so we will denote it by $f(\mathbf{k})$.

As we are interested in the lowest lying excitations of a single monopole, we restrict ourselves to single particle states throughout this analysis; this is a safe assumption so long as we work at long distances.

To determine what we should expect from our lattice simulations, let us evaluate this for the magnetic and scalar field operators. First, let us take our operator to be

$$\hat{\mathcal{O}} = \text{Tr } \hat{\Phi}^2. \quad (8.28)$$

There is no analytic expression for the classical (non-BPS) 't Hooft-Polyakov monopole solution, but in continuum the scalar field has the “hedgehog” form

$$\Phi(r) = \frac{v}{\sqrt{2}} H(r) \frac{\boldsymbol{\sigma} \cdot \mathbf{x}}{r}, \quad (8.29)$$

where $r = |\mathbf{x}|$, and $H(r)$ is a function which approaches 1 at $r \rightarrow \infty$ with the asymptotic behaviour [55]

$$H(r) - 1 \sim \frac{e^{-m_H r}}{m_H r} \quad (8.30)$$

for $m_H < 2m_W$. The Fourier transform of the classical profile $\text{Tr } \Phi^2 = v^2 H(r)^2$ has a delta function peak at $\mathbf{k} = 0$, but otherwise it is finite and approaches a constant value at low momenta

$$\langle \mathbf{k} | \text{Tr } \hat{\Phi}^2 | \mathbf{0} \rangle \sim \frac{M v^2}{m_H^3} \quad \text{as } k \rightarrow 0. \quad (8.31)$$

For more precise comparison, we will use gradient flow to find the classical monopole configuration Φ, U numerically for our chosen lattice sizes. Note that we previously used gradient flow to obtain a classical lattice defect configuration in Chapter 6, but our specific reasons are different here.

Now let us take our operator to be the magnetic field $\mathbf{B}(\mathbf{x})$. This form factor is the most directly measurable quantity characterising magnetic

monopoles, because it determines their scattering amplitude with photons.

We expect for a semiclassical monopole that this will be of the standard Coulomb form,

$$\mathbf{B}(\mathbf{x}) = \frac{1}{g} \frac{\mathbf{x}}{x^3}. \quad (8.32)$$

Then the form factor for a pointlike monopole interacting with the magnetic field is

$$\langle \mathbf{k} | \hat{\mathbf{B}}(0) | 0 \rangle = \frac{M}{g} \int d^3x e^{i\mathbf{k}\cdot\mathbf{x}} \frac{\mathbf{x}}{(x_1^2 + x_2^2 + x_3^2)^{3/2}}. \quad (8.33)$$

Let us choose a basis such that the momentum is now parallel to x_3 . In the magnetic field direction parallel to $\mathbf{k}$, we now have

$$\langle k | \hat{B}_3(0) | 0 \rangle = \frac{M}{g} \int d^3x e^{ikx_3} \frac{x_3}{(x_1^2 + x_2^2 + x_3^2)^{3/2}} \quad (8.34)$$

$$= i \frac{4\pi M}{g} \frac{1}{k}. \quad (8.35)$$

By contrast, in perpendicular directions the integral becomes

$$\langle k | \hat{B}_2(0) | 0 \rangle = \frac{M}{g} \int d^3x e^{ikx_3} \frac{x_2}{(x_1^2 + x_2^2 + x_3^2)^{3/2}}, \quad (8.36)$$

which will give zero. In summary, we have

$$\langle \mathbf{k} | \hat{\mathbf{B}}(0) | 0 \rangle = i \frac{4\pi M}{g} \frac{\mathbf{k}}{k^2}. \quad (8.37)$$

Note that this result is the same as for a pointlike monopole, which means that the semiclassical calculation is not sensitive to the size or internal structure of the monopole in any way. Therefore it is not useful for probing the properties of magnetic monopoles, and one needs a quantum mechanical result instead.

8.4.2 Form factors from two-point functions

Having obtained semiclassical form factors for a pointlike monopole as well as an extended monopole in finite volume, we now look at how to obtain the same quantity from a lattice simulation by adopting the method of the previous chapter generalised to the present case.

Matrix elements like f cannot be computed directly using Monte Carlo simulations. Instead, the basic observable is the field correlation function,

which we consider in the ground state $|0\rangle$ of the one-monopole sector. We work with the magnetic field correlator using the definition of the residual $U(1)$ given in the previous section.

We calculate this correlation function in momentum space, taking the Fourier transform in space but not in the Euclidean time direction, and write a spectral expansion in terms of energy eigenstates $|\alpha\rangle$ with energies E_α ,

$$\langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle = \sum_{\alpha} \frac{\langle 0 | \hat{\mathcal{O}}(\mathbf{k}) | \alpha \rangle \langle \alpha | \hat{\mathcal{O}}(\mathbf{q}) | 0 \rangle}{\langle 0 | 0 \rangle} e^{-t(E_\alpha - E_0)}, \quad (8.38)$$

where $E_0 = M$ is the energy of the single-monopole ground state.

Furthermore, the Euclidean spacetime is necessarily finite in actual Monte Carlo simulations. We denote the length of the system in the time direction by T and in the three space directions by L . We apply twisted boundary conditions (8.8) to the spatial boundaries. In addition to creating an odd magnetic charge, this has the effect that all observables that are odd under charge conjugation such as $\mathbf{B}$ are antiperiodic, and even observables such as $\text{Tr } \Phi^2$ are periodic. Their momenta $\mathbf{k}$ and $\mathbf{q}$ in Eq. (7.10) are therefore also quantised accordingly,

$$k_i = \begin{cases} (2n_i + 1)\pi/L, & \text{for odd operators,} \\ 2n_i\pi/L, & \text{for even operators,} \end{cases} \quad (8.39)$$

with $n_i \in \mathbb{Z}$.

In the time direction, we impose periodic boundary conditions. The correlator can be written as

$$\begin{aligned} \langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle &= \frac{1}{Z} \text{Tr } \hat{U}(T-t) \hat{\mathcal{O}}(\mathbf{q}) \hat{U}(t) \hat{\mathcal{O}}(\mathbf{k}) \\ &= \frac{1}{Z} \sum_{\alpha, \alpha'} \langle \alpha' | \hat{\mathcal{O}}(\mathbf{q}) | \alpha \rangle \langle \alpha | \hat{\mathcal{O}}(\mathbf{k}) | \alpha' \rangle e^{-E_{\alpha'}(T-t) - E_\alpha t}, \end{aligned} \quad (8.40)$$

where $U(t) = \exp(-Ht)$ is the Euclidean time evolution operator, and $Z = \text{Tr } U(T)$.

With twisted boundary conditions, the states $|\alpha\rangle$, $|\alpha'\rangle$ must have odd magnetic charge; because of momentum conservation, they must also have opposite overall momentum $\mathbf{k} = -\mathbf{q}$.

The lowest such state is the single-particle state of a monopole with momentum $\mathbf{k}$, which has energy

$$E_{\mathbf{k}} = \sqrt{k^2 + M^2} \approx M + \frac{k^2}{2M}. \quad (8.41)$$

The next states in the spectrum are two-particle states with a monopole moving at momentum $\mathbf{k}'$ and a photon with momentum $\mathbf{k} - \mathbf{k}'$. In a box of size L , the momentum of the photon is quantised, and therefore there is a large gap $\sim \pi/L \gg k^2/2M$ between the single-particle state and the lowest two-particle state.

At long time separation, we can therefore approximate Eq. (7.14) by an integral over single-particle momentum eigenstates $|\mathbf{k}\rangle$,

$$\begin{aligned} \langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle &= \frac{1}{Z} \int \frac{d^3 k'}{(2\pi)^3 E_{\mathbf{k}'}} \frac{d^3 k''}{(2\pi)^3 E_{\mathbf{k}''}} \langle \mathbf{k}' | \hat{\mathcal{O}}(\mathbf{q}) | \mathbf{k}'' \rangle \langle \mathbf{k}' | \hat{\mathcal{O}}(\mathbf{k}) | \mathbf{k} \rangle e^{-E_{\mathbf{k}'}(T-t) - E_{\mathbf{k}''}t} \\ &= \frac{1}{Z} (2\pi)^3 \delta^{(3)}(\mathbf{q} + \mathbf{k}) \int \frac{d^3 k'}{(2\pi)^3} \frac{|f(\mathbf{k}' - \mathbf{k}, \mathbf{k}')|^2}{E_{\mathbf{k}' - \mathbf{k}} E_{\mathbf{k}'}} e^{-E_{\mathbf{k}'}(T-t) - E_{\mathbf{k}' - \mathbf{k}}t}. \end{aligned} \quad (8.42)$$

Similarly, we can write the partition function as

$$\begin{aligned} Z &= \int \frac{d^3 k'}{(2\pi)^3 E_{\mathbf{k}'}} \langle \mathbf{k}' | \hat{U}(T) | \mathbf{k}' \rangle = L^3 \int \frac{d^3 k'}{(2\pi)^3} e^{-E_{\mathbf{k}'}T} \\ &\approx L^3 \int \frac{d^3 k}{(2\pi)^3} e^{-\left(M + \frac{k^2}{2M}\right)T} = L^3 \left(\frac{M}{2\pi T}\right)^{3/2} e^{-MT}. \end{aligned} \quad (8.43)$$

This partition function is the individual contribution to the partition function from each monopole's worldline in Eq. (8.9), and using Eq. (8.10) it can be written as

$$Z = Z_1 e^{-MT}. \quad (8.44)$$

The integral of Eq. (8.42) has a simple geometrical interpretation: The monopole travels from time 0 to time t at momentum $\mathbf{k}' - \mathbf{k}$, where it absorbs a photon or scalar particle (in line with the schematic of Figure 7.1, but in three dimensions rather than one). This changes the momentum of the monopole to $\mathbf{k}'$, with which it moves forward in time through the periodic boundary back to time 0.

To calculate the integral (8.42), we use the saddle point approximation.

The saddle point $\mathbf{k}_0$ is found by minimising the action

$$S(k') = E_{k'}(T - t) + E_{k'-k}t - MT \quad (8.45)$$

for given t . By approximating the integral by a Gaussian around the saddle point, we obtain

$$\langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle = \frac{1}{Z} (2\pi)^3 \delta^{(3)}(\mathbf{q} + \mathbf{k}) \int \frac{d^3 k'}{(2\pi)^3} \frac{|f(\mathbf{k}' - \mathbf{k}, \mathbf{k}')|^2}{E_{\mathbf{k}' - \mathbf{k}} E_{\mathbf{k}'}} e^{-S(\mathbf{k}_0) - \frac{1}{2}(\mathbf{k}' - \mathbf{k}_0) \cdot \mathbf{M}(\mathbf{k}_0) \cdot (\mathbf{k}' - \mathbf{k}_0)}, \quad (8.46)$$

where $\mathbf{M}(\mathbf{k}_0)$ is the Hessian matrix with components

$$M_{ij}(\mathbf{k}_0) = \left. \frac{\partial^2 S(\mathbf{k}')}{\partial k'_i \partial k'_j} \right|_{\mathbf{k}' = \mathbf{k}_0}. \quad (8.47)$$

By taking t and $T - t$ very large, this forms a nascent delta function. We can use the limit

$$e^{-x^2/a} = \sqrt{a\pi} \delta(x) \quad a \rightarrow 0 \quad (8.48)$$

thus we can calculate the integral

$$\langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle = \frac{1}{Z_1} (2\pi)^3 \delta^{(3)}(\mathbf{q} + \mathbf{k}) \frac{|f(\mathbf{k}_0 - \mathbf{k}, \mathbf{k}_0)|^2}{E_{\mathbf{k}_0 - \mathbf{k}} E_{\mathbf{k}_0}} \frac{1}{(2\pi)^{3/2} W(\mathbf{k}_0)} e^{-S(\mathbf{k}_0)}, \quad (8.49)$$

where

$$W(\mathbf{k}_0) = \sqrt{\det \mathbf{M}(\mathbf{k}_0)}. \quad (8.50)$$

In the non-relativistic limit $k \ll M$, where the form factor is a function of the momentum difference only, we find

$$\langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle \approx \frac{(2\pi)^3 \delta^{(3)}(\mathbf{k} + \mathbf{q})}{L^3} \left(\frac{T}{M} \right)^{3/2} \frac{|f(\mathbf{k})|^2}{E_{\mathbf{k}_0 - \mathbf{k}} E_{\mathbf{k}_0} W(k_0)} e^{-S(\mathbf{k}_0)}, \quad (8.51)$$

where we have substituted the expression (8.10) for Z_1 .

We can use Eq. (8.51) to determine the form factor from the field cor-

relator. For given $\mathbf{k}$ and t , we obtain the saddle point $\mathbf{k}_0$ by minimising Eq. (7.19), and the form factor is finally given by

$$f(\mathbf{k}) = \pm i \sqrt{\langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, -\mathbf{k}) \rangle} \times \left(\frac{M}{T} \right)^{3/4} \sqrt{E_{\mathbf{k}_0 - \mathbf{k}} E_{\mathbf{k}_0} W(k_0)} e^{S(\mathbf{k}_0)/2} \quad (8.52)$$

for $\mathcal{O}$ odd. The factor of i is not present for even operators, due to parity considerations.

8.4.3 Mass measurements

The time separation t enters into Eq. (8.52) directly – in parameterising the two-point function – as well as indirectly, in the saddle-point calculation for $\mathbf{k}_0$. However, since $\mathbf{k} \ll M$ in the current calculation we can take the nonrelativistic limit of the action in Eq. (8.45) and let $\mathbf{k}_0 = \mathbf{k}t/T$ for arbitrary t . To order $\mathbf{k}$, there are no t -dependent quantities outside of the action in our expression for the form factor. Thus, as expected, at low momenta we effectively have

$$\langle \mathcal{O}(0, \mathbf{k}) \mathcal{O}(t, \mathbf{q}) \rangle = \frac{|f|^2}{M^2} e^{-\sqrt{M^2 + k_0(t)^2}t - \sqrt{M^2 + (k - k_0(t))^2}(T-t) + MT}. \quad (8.53)$$

We can use this result to conduct a fit to the correlator, noting that this is merely one contribution to the two-point function; the other most significant contribution (particularly at shorter distances) will be from the lightest particle that the operator $\mathcal{O}$ can create propagating in the bulk. Hence, if we take $\mathcal{O} = B_i$ then this will be the photon, which we will treat as massless; for $\mathcal{O} = \text{Tr } \Phi^2$ it will be the bulk scalar particle, which has a mass $m_H = \sqrt{2}|m|$.

As always, we are assuming in using this calculation that the particles created by the correlation function either interact directly with the monopole, propagate solely in the bulk, or are annihilated by the vacuum.

8.5 Results

Simulations were carried out using a $16^3 \times 48$ lattice with $\lambda = 0.1$ and $g = 1/\sqrt{5}$.

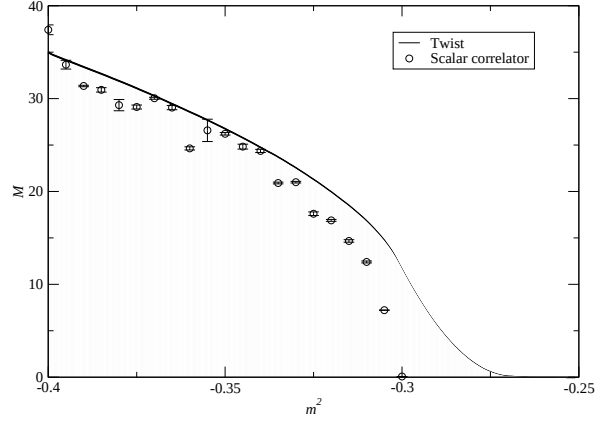


Figure 8.2: Plot of the monopole mass obtained from the scalar field correlator, with twist measurement overplotted for comparison. The scalar field correlator with $\mathbf{k} = (2\pi/L, 0, 0)$ and permutations is used, the lowest permitted nonzero momentum.

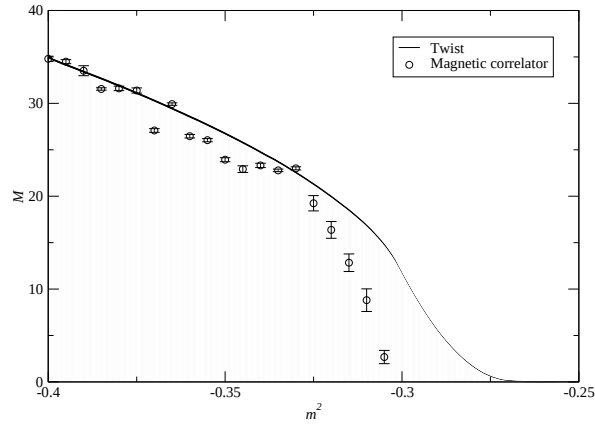


Figure 8.3: Plot of the monopole mass obtained from the magnetic field correlator, with twist measurement overplotted for comparison. The momenta used are $\mathbf{k} = (3\pi/L, \pi/L, \pi/L)$, and permutations. The results are similar to the scalar field case.

Configurations were created by generating a classical ‘cold’ monopole and then ‘heating’ the configuration gradually towards the phase transition. Once thermalisation of $\text{Tr } \Phi^2$ had occurred for a given parameter choice, the resulting configuration was used as the input for the next value of m^2 closer to the phase transition. In this way, a set of configurations was generated which could then be simulated separately.

We thermalised the system initially deep in the broken phase, and then gradually increasing the value of m^2 . As we discussed in Chapter 1, moving through the phase transition in the opposite direction produces extra monopoles which would take a very long time to annihilate [85, 122].

The system seems very susceptible to the creation of metastable states, particularly long-lived monopole-antimonopole pairs as well as what appeared to be excited states of the monopole. After thermalisation of $\text{Tr } \Phi^2$, additional checks on the histogram of total charge of the system were carried out; fluctuations due to the finite volume (indicated by Eq. 8.9) were to be expected, but any skewness in the distribution led us to reject the thermalisation and try again. For these reasons it proved very difficult to start from the symmetric phase or attempt to study the monopole mass using hysteresis curves.

8.5.1 Mass measurements and comparison

Three methods were used to attempt to measure the mass of the monopole. The first was the well-established response to a twist obtained from Eq. (8.16), and used previously in Ref. [123]; we also made use of it as a comparator in Chapter 6. The lattices in that work were considerably smaller in the Euclidean time direction but the response to a twist measured here is in good agreement with the $L = 16$ data that were obtained. The measurements are plotted as a continuous line in both Figures 8.2 and 8.3, for reasons discussed at length in Section 8.3. The thickness of the line is the estimated error.

It was found that, for the histograms to offer sufficient overlap that the free energy estimates (8.20) and (8.21) agreed within errors, a measurement spacing of at most $\delta m^2 = 0.001$ was required. The solid line plotted therefore required in excess of 150 separate simulations to keep systematic errors below 2σ , although f_1 is consistently lower than f_2 .

The twist measurements clearly have a finite size effect (also seen in Ref. [123]) that affects the measurements of the monopole mass when the physical size of the monopole almost fills the box. The curve of the twist results changes concavity as the monopole becomes smaller than the box size, and deeper in the broken phase the monopole mass behaves in a manner similar to the classical monopole mass.

The errors were obtained using the methods described in Section 8.3. No attempt was made to account for the nonzero covariance between adjacent mass interval measurements, but it is felt that this would not give a major systematic contribution to the error.

Let us now turn our attention to the use of the two-point correlator to calculate masses as described in Section 8.4.3. We carried out a fit to Eq. (8.53), plus a bulk field which we expect will be either the scalar or the photon, depending on the operator used:

$$C(t) = C_1 e^{-\sqrt{M^2+k_0(t)^2}t-\sqrt{M^2+(k-k_0(t))^2}(T-t)+MT} + C_2 \left(e^{-E_{\text{bulk}}t} + e^{-E_{\text{bulk}}(T-t)} \right). \quad (8.54)$$

To ensure that our error estimates are robust despite the clear correlations between data points at different separations exhibited by the two-point function, we use a jackknifed nonlinear least squares fit method. The error estimates obtained from this technique are (in the present work) in agreement with those from our previous use of bootstrapping, but there exist results demonstrating the robustness of the jackknife technique for residuals that are not independently and identically distributed [134].

The length of each simulation run was about ten to twenty times that for each simulation used in the response to a twist technique discussed above. On the other hand, for the single point at $m^2 = -0.4$, the results of 150 such simulations in two topological sectors are required for the twist calculation (given the conditions above of a spacing where the two measurements f_1 and f_2 agree to within 2σ), whereas just one measurement in the topologically nontrivial sector is needed with the correlator calculation. Added to this is the task of thermalising every one of those 300 ensembles and avoiding metastability. Therefore, it is simulationally less demanding to use the correlator measurement deep in the broken phase – if it can be relied upon. Close to the phase transition, the finite size effects of either technique are

severe in such a small box. We must therefore leave it to future work to study the dynamics of quantum monopoles at strong coupling near the critical point [123].

Based on Figure 8.2, it seems that there is a very small systematic discrepancy between the twist and correlator results when the correlator of the scalar field is used. Given the relatively small lattice sizes used, it is not inconceivable that this is due to the finite size effect in one of the two quantities measured, but long-lived metastable states are another possibility. Note that we do not anticipate any major lattice artefacts playing a role in the monopole dynamics until $m_H \approx 1$, when the scalar mass is about the reciprocal lattice spacing, at which time the monopole will become small enough to feel the potential due to the discretised lattice more severely [142].

The results for the magnetic field correlator are shown in Figure 8.3. Since the magnetic field operator couples to the photon, we anticipate that part of the signal in this case comes from a massless photon field propagating in the bulk. This assumption seems borne out by the failure of our fitting ansatz for $\mathbf{k} = (\pi/L, \pi/L, \pi/L)$, and the need to go to $\mathbf{k} = (3\pi/L, \pi/L, \pi/L)$ to see the correlator expected of the monopole signal.

Despite the apparent systematic discrepancy, the fits yielding the data for Figure 8.3 are very good, and the form of the correlator given in Eq. (8.53) seems to be the right one; the long distance ‘plateau’ behaviour is a good fit.

8.5.2 Form factor measurements

Having studied the mass using the low-momentum correlator measurements, we now move on to the form factor measurements. From the results of the Monte Carlo simulations we use Eq. (8.52) to obtain the form factor, and compare with semiclassical expectations. To minimise sources of systematic error, we use the twist results for the value of M in computing form factors.

We start by looking at the scalar field form factor $f_\Phi(k) = \langle \mathbf{k} | \text{Tr } \hat{\Phi}^2 | \mathbf{0} \rangle$ for which there is a semiclassical comparison available, albeit not in analytic form. We obtain the classical monopole configuration on the lattice using gradient flow. According to Eq. (8.27), the form factor can then be recovered by Fourier transforming $\text{Tr } \Phi^2$, for comparison with the measurement from the Monte Carlo simulation.

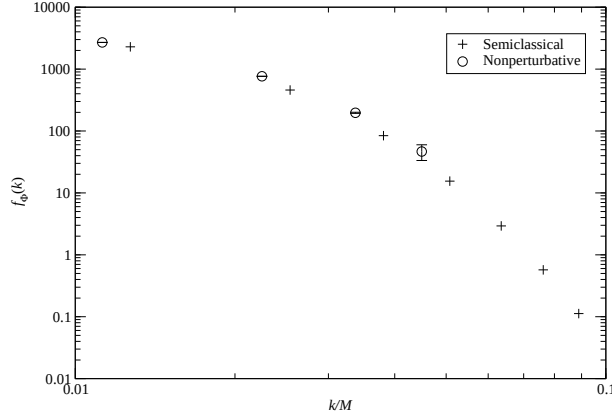


Figure 8.4: Plot of the monopole form factor for the scalar field $f_\Phi(k)$. The measurement is deep in the broken phase with $m^2 = -0.4$. For comparison, the semiclassical result is also shown; renormalisation conditions have been used such that the vacuum expectation value for the gradient flow monopole matches that measured in the nonperturbative simulation; its classical mass is then $M_{\text{cl}} = 30.9$, to be compared with $M = 34.9 \pm 0.1$ for the quantum monopole.

The minimisation was started from a classical ‘hedgehog’ $\phi^i(\mathbf{x}) \propto \mathbf{x} \cdot \hat{\mathbf{i}}$ with a trivial gauge field $U_\mu(x) = 1$. A local minimum of the Euclidean action was obtained using

$$\begin{aligned} \phi^a(x, \tau + \delta\tau) = \phi^a(x, \tau) + \delta\tau \Bigg[& - \left[4(8 + m^2) + 8\lambda \text{Tr } \Phi^2 \right] \phi^a(x, \tau) \\ & + \sum_j \left[\sigma^a U_j(x, \tau) \Phi(x + \hat{j}, \tau) U_j^\dagger(x, \tau) \right] \Bigg] \quad (8.55) \end{aligned}$$

and

$$\begin{aligned}
U_i(x, \tau + \delta\tau) = \exp i \delta t \sigma^a \Bigg[& - \frac{\beta}{2} \sum_{\text{staple}} \text{Tr} \{ \sigma^a U_{ij}(x, \tau) \} \\
& + 2 \text{Tr} \left\{ \sigma^a U_i(x, \tau) \Phi(x, \tau) U_i^\dagger(x, \tau) \Phi(x + \hat{i}, \tau) \right. \\
& \left. - \text{h.c.} \right\} \Bigg] U_i(x, \tau). \quad (8.56)
\end{aligned}$$

The length T of the Euclidean time direction is not relevant for this process and so we could set $T = 1$. The resulting field configurations were used to obtain the scalar field $\text{Tr} \Phi^2$ in the presence of the classical monopole. As a by-product the classical mass was obtained (for comparison with the twist results above), by looking at the difference in energy between topologically trivial and topologically nontrivial configurations,

$$M_{\text{cl}}(m^2) = E_{\text{tw}}(m^2) + \frac{m^4}{4\lambda} L^3. \quad (8.57)$$

Our results deep in the broken phase are shown in Figure 8.4. In this plot, a single value of $m^2 = -0.4$ has been used for the Monte Carlo simulations, and the classical monopole with the closest matching mass was used for the comparison. There is, unsurprisingly, good agreement between the two. The semiclassical agreement demonstrates that our technique generalises reliably from the relatively straightforward case of the kink to higher dimensions.

The magnetic field form factor $\mathbf{f}_{\mathbf{B}}(\mathbf{k}) = \langle \mathbf{k} | \hat{\mathbf{B}} | 0 \rangle$, is perhaps physically more interesting. It is a vector quantity, but in continuum its direction is always parallel to $\mathbf{k}$ because of rotation invariance, and therefore only its length $f_{\mathbf{B}}(k) = |\mathbf{f}_{\mathbf{B}}(\mathbf{k})|$ is non-trivial. On the other hand, in the simulations it is easiest to consider its individual components $[\mathbf{f}_{\mathbf{B}}(\mathbf{k})]_i$, but because of the boundary conditions we cannot choose the momentum to be parallel to a coordinate axis. Instead, we note that the length of the vector can be written as

$$f_{\mathbf{B}}(k) = \frac{k}{k_i} [\mathbf{f}_{\mathbf{B}}(\mathbf{k})]_i. \quad (8.58)$$

This quantity is shown for various values of m^2 and k in Figure 8.5. For $k \ll m_H$, we are probing wavelengths longer than the monopole core size, and therefore the curve approaches the expected Coulomb result of Eq. (8.37). In the semiclassical calculation this behaviour extends to arbitrarily high

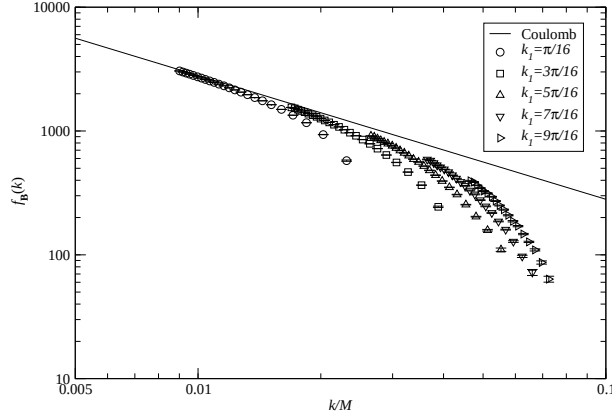


Figure 8.5: Plot of the monopole form factor for the magnetic field $f_{\mathbf{B}}(k)$, for momenta $(k_1, \pi/L, \pi/L)$ and permutations on a doubly logarithmic scale. The comparison is with the Coulomb result.

momenta, which corresponds to a pointlike charge, but our results show that in the quantum theory there is a clear deviation from the Coulomb result at shorter wavelengths, when $k \gtrsim m_H$. One interpretation for this is that because of quantum fluctuations, the magnetic charge is spread out over distance $\sim 1/m_H$.

In Figure 8.6, we highlight two fixed values of m^2 and plot the form factor for various values of k . Changing the value of m^2 can be interpreted as changing the physical lattice spacing. Moving closer to the critical point, i.e., towards higher m^2 , corresponds to taking the continuum limit. In Figure 8.6, we see that closer to the continuum limit, the charge distribution becomes more spread out in physical units. On physical grounds we would expect that it approaches a finite continuum limit.

8.5.3 A note on algorithms and performance

Previous nonperturbative studies of topological solitons have typically employed a standard Metropolis update algorithm. It would seem, however, that excitations corresponding to an extended defect's worldline are not going to be quickly thermalised or decorrelated by updates that are local

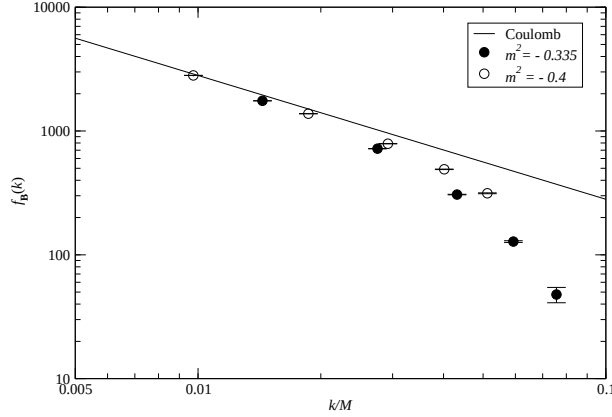


Figure 8.6: Plot of the monopole form factor for the magnetic field $f_{\mathbf{B}}(k)$, for $m^2 = -0.335$ and $m^2 = -0.4$, which can be interpreted as two different lattice spacings. The Coulomb result is again included for comparison.

in space. Indeed, the classical topological soliton is a solution of the field equations, so an obvious way to improve ergodicity would seem to be to use one of the family of algorithms which relies on real-time dynamics. For this reason, despite the added computational cost – and the complexity arising from the twisted boundary conditions – it was decided to investigate the performance of a Hybrid Monte Carlo (HMC) algorithm (see Section 5.1.1). This showed promise in the previous chapter when fighting critical slowing down in our studies of the form factors of critical kinks, despite clear disadvantages to using HMC with scalar fields in general. We hypothesised that this was due to the fact that the defects obey the equations of motion, and so using an update method that integrates the equations of motion (or a generalisation thereof) improves ergodicity for observables associated with the quantum topological soliton. In contrast, a single Metropolis update step will not significantly alter the position or configuration of a topological defect.

In the current situation, however, it was difficult to detect an advantage to using HMC. While the autocorrelation time was in many cases the same, the CPU time required to integrate a single trajectory was longer than a

single Metropolis checkerboard sweep; the staples must be recalculated for every step in the trajectory. This may be due to our being at relatively weak coupling, with severe finite size effects that mask any critical slowing down. It may also be due to inadequate tuning of the HMC algorithm to give an optimal acceptance rate.

Lastly, to improve statistics for the magnetic field correlator we considered an overrelaxation step for the $SU(2)$ gauge fields, coupled to an accept-reject step to account for the covariant derivative term in the action. We made use of the $SU(2)$ move $U \rightarrow U_0 U^{-1} U_0$. This leaves the Wilson term unchanged when $U_0 = S^{-1} \sqrt{\det S}$, where S is the ‘staple’ [30]. Unfortunately we did not notice any substantial improvement to the statistics as a result of adding this step.

8.6 Summary

We have used correlation functions to measure properties of the ’t Hooft-Polyakov monopole nonperturbatively. For the monopole mass we found good agreement with previous studies that used the response to twisted boundary conditions.

We also calculated the form factors of the monopole for scalars and photons. For the scalar we find good agreement with the semiclassical results, which was expected because of the weak coupling. In contrast, the semiclassical result for the photon is that of a point particle, but the quantum result shows smooth internal structure. This shows that a proper quantum calculation is absolutely necessary in order to probe the internal structure of monopoles using photons [41]. The continuum limit deserves to be explored using the same techniques. We should also bear in mind that although our expression Eq. (8.6) for the magnetic field has attractive properties, it is not the exact creation operator for asymptotic photon states in the full quantum theory. In principle, a numerical approximation for the correct creation operator could be obtained by a diagonalisation procedure.

In Ref. [45], it was shown how to generalise the twisted boundary conditions to other $SU(N)$ +Higgs models, N even. Although odd N is arguably of greater phenomenological interest, the techniques here should be equally valid in these cases.

9 Conclusions

In this thesis, we have sought to use nonperturbative methods from lattice quantum field theory to study the properties of topological solitons. Applying twisted spatial boundary conditions to create the solitons, we studied their interactions, excitations and dispersion relation.

As there are very few perturbative results for topological solitons, it is very difficult to study such matters analytically. It is possible to do so when the defects are integrable, but the models which were of interest to us here do not have that property. We did, however, demonstrate agreement in Chapter 7 with the form factor for an exactly solvable model (the 2D Ising model).

Our use of correlation functions, rather than just measuring free energies as a response to a twist, is the single major novel contribution in this thesis. While most of the methods used here (with the exception of our form factor calculations) are adaptations of techniques used in other situations in lattice field theory, our use of them to study the behaviour of topological solitons is completely new. Furthermore, the form factor calculations bear little resemblance to previous lattice field theory studies and can be seen as offering a completely new direction of study.

The first half of the thesis – Chapters 1 to 5 – consisted of introductory material. We put the study of the quantum properties of topological solitons into its wider context, and elucidated the properties of classical topological solitons. We proceeded with their perturbative quantisation (demonstrating the limitations of that technique). Next, we moved on to introduce the rudiments of lattice field theory and some of the simulational techniques that can be used.

We then developed these techniques – those adapted from other work in lattice quantum field theory, as well as the form factor measurements which are completely new, in Chapters 6 and 7. Here we applied them to a toy model, the $\lambda\phi^4$ kink, and demonstrated successfully that they work and give

the correct results in various limits.

In more complicated theories, things are less straightforward. For example, one will obtain several form factors which describe interactions of the soliton with different particle species. In the case of point-like solitons, such as 't Hooft-Polyakov monopoles in 3+1-dimensional gauge field theory, the calculation proceeded successfully along the same lines. The results of this work were discussed in Chapter 8.

To summarise, we have demonstrated that it is possible to use correlators in field theories with twisted boundary conditions to study the energies, dispersion relations and excitations of topological solitons. We have also developed new techniques to study their form factors.

9.1 Directions for future work

It would be interesting to study dyons and other excitations of 't Hooft-Polyakov monopoles, and localisation of degrees of freedom on cosmic strings, domain walls or solitonic branes in braneworld models. These studies would involve a generalisation of the two-particle operator techniques described in Chapter 6. In many cases, a detailed understanding of the particle spectrum for the theory in the presence of a defect would also be obtainable using these techniques.

The form factor approach to studying topological solitons means that, at the quantum level, we must accept that no unambiguous notion of 'width' or 'size' can be considered for a given scattering process. Hence, we would also propose using the form factor as an observable in the study of confining flux tubes instead of probe plaquettes [60].

We have already mentioned that other theories possessing kink solutions (such as the sine-Gordon model) can be investigated using the same techniques, as can other topological solitons. Some models are currently under investigation [11, 91].

The study of 't Hooft-Polyakov monopoles on the lattice has been shown to be possible for $SU(N)$ when N is even in Ref. [45], but it is the N odd cases ($SU(3)$ and $SU(5)$) that are perhaps of greatest phenomenological interest. There is also the theoretical question of whether it is possible to implement twisted boundaries in such circumstances at all.

Generalisation to extended defects, such as domain walls, strings or higher-

dimensional membranes should be straightforward. For example, this will make it possible to study non-perturbatively the quantum mechanical properties and interactions of cosmic strings; this would appear to be an important future direction of study.

One possibility would be to use the techniques presented here to study the defects present in supersymmetric theories such as the Wess-Zumino Model or SQCD and hence as a test of lattice supersymmetry [59].

Can we relate lattice results to monopole pair production rates? Phenomenologically, this would be very important [41]. Unfortunately, what we have been calculating in this thesis relates to scattering of a soliton off a particle rather than soliton pair creation; the differences are perhaps more profound than they at first appear.

In summary, then, there are perhaps two directions in which the calculations could be taken further. One could apply the same ideas to other models, or instead seek to relate what has been measured and studied here more closely to other aspects of theoretical physics.

Bibliography

- [1] ABRAHAM, D. (1986) Surface structures and phase transitions – exact results. In *Phase Transitions and Critical Phenomena, Vol. 10*, chap. 1 (Academic Press).
- [2] ALEXANDRE, J. and FARAKOS, K. (2008) Path integral quantization of scalar fluctuations above a kink. *J. Phys.* **A41**, 015401.
- [3] ARDEKANI, A. and WILLIAMS, A. G. (1999) Lattice study of the kink soliton and the zero-mode problem for ϕ^4 in two dimensions. *Austral. J. Phys.* **52**, 929. [arXiv:hep-lat/9811002](#).
- [4] ARNOLD (1904) *The letter of Petrus Peregrinus on the Magnet, A.D. 1269* (McGraw Publishing Company, New York).
- [5] BALL, R. D. (1990) Mesons, Skyrmions and baryons. *Int. J. Mod. Phys.* **A5**, 4391.
- [6] BENDER, C. M., FEINBERG, J., HOOK, D. W. and WEIR, D. J. (2009) Chaotic systems in complex phase space. *Pramana* **73**, 453. [arXiv:0809.1975](#).
- [7] BERG, B., KAROWSKI, M. and WEISZ, P. (1979) Construction of Green functions from an exact S matrix. *Phys. Rev.* **D19**, 2477.
- [8] BERGES, J. and ROTH, S. (2011) Topological defect formation from 2PI effective action techniques. *Nucl. Phys.* **B847**, 197. [arXiv:1012.1212](#).
- [9] BESSA, A., DE CARVALHO, C. A. A. and FRAGA, E. S. (2004) Correlations around an interface. *Phys. Rev.* **D69**, 125013.
- [10] BEVIS, N., HINDMARSH, M., KUNZ, M. and URRESTILLA, J. (2008) Fitting CMB data with cosmic strings and inflation. *Phys. Rev. Lett.* **100**, 021301.

- [11] BITKEVICIUS, L. (2011) *Numerical approach to the non-perturbative mass of a quantum sine-Gordon soliton in (1+1) dimensions*. Master's thesis, Imperial College London.
- [12] BOGOMOLNY, E. B. (1976) Stability of classical solutions. *Sov. J. Nucl. Phys.* **24**, 449.
- [13] BORDAG, M., GOLDHABER, A. S., VAN NIEUWENHUIZEN, P. and VASSILEVICH, D. (2002) Heat kernels and zeta-function regularization for the mass of the SUSY kink. *Phys. Rev.* **D66**, 125014. [arXiv:hep-th/0203066](#).
- [14] BORN, M., STOYLE, R. J. B. and RADCLIFFE, J. M. (1990) *Atomic Physics (8th Ed.)* (Dover Publications).
- [15] BRADEN, H. W. (1987) Mass corrections to periodic solitons. *J. Math. Phys.* **28**, 929.
- [16] BURSA, F. and TEPER, M. (2005) Casimir scaling of domain wall tensions in the deconfined phase of $D = 3 + 1$ $SU(N)$ gauge theories. *J. High Energy Phys.* **08**, 060.
- [17] CALZETTA, E. and HU, B. (2008) *Nonequilibrium Quantum Field Theory* (Cambridge University Press, Cambridge).
- [18] CAMPBELL, D. K., SCHONFELD, J. F. and WINGATE, C. A. (1983) Resonance Structure in Kink - Antikink Interactions in ϕ^4 Theory. *Physica* **9D**, 1.
- [19] CARRIGAN, R. A., (ED.) and TROWER, W. P., (ED.) (1983) Magnetic monopoles. *NATO Adv. Study Inst. Ser. B Phys.* **102**, 1.
- [20] CASELLE, M., HASENBUSCH, M. and PROVERO, P. (1999) Non-perturbative states in the 3D ϕ^4 theory. *Nucl. Phys.* **B556**, 575.
- [21] CHRIST, N. H. and LEE, T. D. (1975) Quantum expansion of soliton solutions. *Phys. Rev.* **D12**, 1606.
- [22] CHUANG, I., YURKE, B., DURRER, R. and TUROK, N. (1991) Cosmology in the laboratory: defect dynamics in liquid crystals. *Science* **251**, 1336.

- [23] CIRAC, J. I. and VERSTRAETE, F. (2009) Renormalization and tensor product states in spin chains and lattices. *Journal of Physics A: Mathematical and Theoretical* **42** 50, 504004.
- [24] CIRIA, J. C. and TARANCON, A. (1994) Renormalization group study of the soliton mass on the $\lambda\phi^4$ in (1+1)-dimensions lattice model. *Phys. Rev.* **D49**, 1020.
- [25] COLEMAN, S. (1985) *Aspects of symmetry: selected Erice lectures* (Cambridge University Press, Cambridge).
- [26] COLEMAN, S. R. (1975) Quantum sine-Gordon equation as the massive Thirring model. *Phys. Rev.* **D11**, 2088.
- [27] CREUTZ, M. Monte Carlo algorithms for lattice gauge theory (lecture notes; technical report BNL-39747).
- [28] CREUTZ, M. (1980) Monte Carlo study of quantized SU(2) gauge theory. *Phys. Rev.* **D21**, 2308.
- [29] CREUTZ, M. (1983) *Quarks, gluons and lattices* (Cambridge University Press, Cambridge).
- [30] CREUTZ, M. (1987) Overrelaxation and Monte Carlo simulation. *Phys. Rev.* **D36**, 515.
- [31] DASHEN, R. F., HASSLACHER, B. and NEVEU, A. (1974) Nonperturbative methods and extended hadron models in field theory. 1. Semiclassical functional methods. *Phys. Rev.* **D10**, 4114.
- [32] DASHEN, R. F., HASSLACHER, B. and NEVEU, A. (1974) Nonperturbative methods and extended hadron models in field theory. 2. Two-dimensional models and extended hadrons. *Phys. Rev.* **D10**, 4130.
- [33] DAVIS, A. C., HART, A., KIBBLE, T. W. B. and RAJANTIE, A. (2002) The monopole mass in the three-dimensional Georgi-Glashow model. *Phys. Rev.* **D65**, 125008. [arXiv:hep-lat/0110154](#).
- [34] DAVIS, A. C., KIBBLE, T. W. B., RAJANTIE, A. and SHANAHAN, H. (2000) Topological defects in lattice gauge theories. *J. High Energy Phys.* **11**, 010.

- [35] DE FORCRAND, P., D'ELIA, M. and PEPE, M. (2001) A study of the 't Hooft loop in SU(2) Yang-Mills theory. *Phys. Rev. Lett.* **86**, 1438. [arXiv:hep-lat/0007034](#).
- [36] DE FORCRAND, P. and PHILIPSEN, O. (2000) Adjoint string breaking in 4d SU(2) Yang-Mills theory. *Phys. Lett.* **B475**, 280. [arXiv:hep-lat/9912050](#).
- [37] DEGRAND, T. and DETAR, C. E. Lattice methods for quantum chromodynamics New Jersey, USA: World Scientific (2006) 345 p.
- [38] DEL CAMPO, A., DE CHIARA, G., MORIGI, G., PLENIO, M. B. and RETZKER, A. (2010) Structural defects in ion crystals by quenching the external potential: the inhomogeneous Kibble-Zurek mechanism. *ArXiv e-prints* [arXiv:1002.2524](#).
- [39] DERRICK, G. H. (1964) Comments on nonlinear wave equations as models for elementary particles. *J. Math. Phys.* **5**, 1252.
- [40] DIRAC, P. A. M. (1931) Quantised singularities in the electromagnetic field. *Proc. Roy. Soc. Lond.* **A133**, 60.
- [41] DRUKIER, A. K. and NUSSINOV, S. (1982) Monopole pair creation in energetic collisions: is it possible? *Phys. Rev. Lett.* **49**, 102.
- [42] DUANE, S., KENNEDY, A. D., PENDLETON, B. J. and ROWETH, D. (1987) Hybrid Monte Carlo. *Phys. Lett.* **B195**, 216.
- [43] DUNNE, G. V. and FEINBERG, J. (1998) Self-isospectral periodic potentials and supersymmetric quantum mechanics. *Phys. Rev.* **D57**, 1271. [arXiv:hep-th/9706012](#).
- [44] DVALI, G. R., GABADADZE, G. and PORRATI, M. (2000) 4D gravity on a brane in 5D Minkowski space. *Phys. Lett.* **B485**, 208. [arXiv:hep-th/0005016](#).
- [45] EDWARDS, S., MEHTA, D., RAJANTIE, A. and VON SMEKAL, L. (2009) 't Hooft-Polyakov monopoles in lattice SU(N)+adjoint Higgs theory. *Phys. Rev.* **D80**, 065030. [arXiv:0906.5531](#).
- [46] EFRON, B. (1982) *The Jackknife, the Bootstrap and other resampling plans* (Society for Industrial and Applied Mathematics).

- [47] EHRMAN, J. R., FOSDICK, L. D. and HANDSCOMB, D. C. (1960) Computation of order parameters in an ising lattice by the monte carlo method. *J. Math. and Phys.* **1** 6, 547.
URL <http://dx.doi.org/doi/10.1063/1.1703692>
- [48] ENDRES, M. G. (2007) Method for simulating $O(N)$ lattice models at finite density. *Phys. Rev.* **D75**, 065012. [arXiv:hep-lat/0610029](#).
- [49] FAIRBAIRN, M. *et al.* (2007) Stable massive particles at colliders. *Phys. Rept.* **438**, 1. [arXiv:hep-ph/0611040](#).
- [50] FENNEL, T., DEEN, P. P., WILDES, A. R., SCHMALZL, K., PRABHAKARAN, D., BOOTHROYD, A. T., ALDUS, R. J., MCMORROW, D. F. and BRAMWELL, S. T. (2009) Magnetic Coulomb phase in the spin ice $\text{Ho}_2\text{Ti}_2\text{O}_7$. *Science* **326**, 415. [arXiv:0907.0954](#).
- [51] FERRENBURG, A. M. and SWENDSEN, R. H. (1988) New Monte Carlo technique for studying phase transitions. *Phys. Rev. Lett.* **61**, 2635.
- [52] FEYNMAN, R. and HIBBS, A. (1965) *Quantum mechanics and path integrals* (McGraw-Hill).
- [53] FINKELSTEIN, D. and MISNER, C. W. (1959) Some new conservation laws. *Annals Phys.* **6**, 230.
- [54] FISHER, M. E. (1984) Walks, walls, wetting, and melting. *Journal of Statistical Physics* **34**, 667.
- [55] FORGACS, P., OBADIA, N. and REUILLON, S. (2005) Numerical and asymptotic analysis of the 't Hooft-Polyakov magnetic monopole. *Phys. Rev.* **D71**, 035002. [arXiv:hep-th/0412057](#).
- [56] FRIEDBERG, R. and CAMERON, J. E. (1970) Test of the monte carlo method: Fast simulation of a small ising lattice **52** 12, 6049.
- [57] GEORGI, H. and GLASHOW, S. L. (1974) Unity of All Elementary Particle Forces. *Phys. Rev. Lett.* **32**, 438.
- [58] GIACOMELLI, G. and PATRIZII, L. (2005) Magnetic monopole searches [arXiv:hep-ex/0506014](#).

- [59] GIEDT, J. (2006) Advances and applications of lattice supersymmetry. *PoS LAT2006*, 008. [arXiv:hep-lat/0701006](#).
- [60] GLIOZZI, F., PEPE, M. and WIESE, U. J. (2010) The Width of the Confining String in Yang-Mills Theory. *Phys. Rev. Lett.* **104**, 232001. [arXiv:1002.4888](#).
- [61] GOCKELER, M., KASTRUP, H. A., WESTPHALEN, J. and ZIMMERMANN, F. (1994) Scattering phases on finite lattices in the broken phase of the four-dimensional $O(4)$ ϕ^4 theory. *Nucl. Phys.* **B425**, 413.
- [62] GODDARD, P. and OLIVE, D. I. (1978) New developments in the theory of magnetic monopoles. *Rept. Prog. Phys.* **41**, 1357.
- [63] GOLDSTONE, J. and JACKIW, R. (1975) Quantization of nonlinear waves. *Phys. Rev.* **D11**, 1486.
- [64] GOLUBCHIK, D., POLTURAK, E. and KOREN, G. (2009) Correlations beyond the horizon. *ArXiv e-prints* [arXiv:0911.5613](#).
- [65] GOODBAND, M. and HINDMARSH, M. (1995) Bound states and instabilities of vortices. *Phys. Rev.* **D52**, 4621. [arXiv:hep-ph/9503457](#).
- [66] GOODBAND, M. and HINDMARSH, M. (1995) Instabilities of electroweak strings. *Phys. Lett.* **B363**, 58.
- [67] GROENEVELD, J., JURKIEWICZ, J. and KORTHALS ALTES, C. P. (1981) Twist as a probe for phase structure. *Phys. Scripta* **23**, 1022.
- [68] HAAR, H. (1933) Der Massbegriff in der Theorie der Kontinuierlichen Gruppen. *Ann. Math. (2)* **34**, 147.
- [69] HAEGEMAN, J., PIRVU, B., WEIR, D. J., CIRAC, J. I., OSBORNE, T. J., VERSCHELDE, H. and VERSTRAETE, F. (2011) A variational matrix product ansatz for dispersion relations. *ArXiv e-prints* [arXiv:1103.2286](#).
- [70] HARDIN, R., SLOANE, N. and SMITH, W. (2000) Tables of Spherical Codes with Icosahedral Symmetry (accessed 2011-08-25).
URL <http://www2.research.att.com/njas/icosahedral.codes/>
- [71] HECHT, E. (2002) *Optics, 4th. Ed* (Addison Wesley, San Francisco).

- [72] HENDRY, P. C., LAWSON, N. S., LEE, R. A. M., MCCLINTOCK, P. V. E. and WILLIAMS, C. D. H. (1994) Generation of defects in superfluid ^4He as an analogue of the formation of cosmic strings. *Nature* **368**, 315.
- [73] HERNANDEZ, P. (2009) Les Houches lectures on lattice field theory .
- [74] HÍJAR, H. and SUTMANN, G. (2008) Monte Carlo estimates of interfacial tension in the two-dimensional Ising model from non-equilibrium methods. *Journal of Statistical Mechanics: Theory and Experiment* **2008** 07, P07012 (22pp).
- [75] HINDMARSH, M. and RAJANTIE, A. (2000) Defect formation and local gauge invariance. *Phys. Rev. Lett.* **85**, 4660. [arXiv:cond-mat/0007361](#).
- [76] HURD, C. C. (1985) A note on early Monte Carlo computations and scientific meetings. *IEEE Ann. Hist. Comput.* **7**, 141.
- [77] JACKIW, R. (1977) Quantum meaning of classical field theory. *Rev. Mod. Phys.* **49**, 681.
- [78] JACKIW, R. and WOO, G. (1975) Semiclassical scattering of quantized nonlinear waves. *Phys. Rev.* **D12**, 1643.
- [79] JELLEY, N. A. (1990) *Fundamentals of Nuclear Physics* (Cambridge University Press, Cambridge).
- [80] KAJANTIE, K., KARKKAINEN, L. and RUMMUKAINEN, K. (1991) Tension of the interface between two ordered phases in lattice SU(3) gauge theory. *Nucl. Phys.* **B357**, 693.
- [81] KAJANTIE, K., LAINE, M., RUMMUKAINEN, K. and SHAPOSHNIKOV, M. E. (1997) 3d SU(N) + adjoint Higgs theory and finite-temperature QCD. *Nucl. Phys.* **B503**, 357. [arXiv:hep-ph/9704416](#).
- [82] KAJANTIE, K. *et al.* (1999) Vortex tension as an order parameter in three-dimensional $U(1)$ + Higgs theory. *Nucl. Phys.* **B546**, 351.
- [83] KAPLAN, D. B. (2009) Chiral symmetry and lattice fermions [arXiv:0912.2560](#).

- [84] KENNEDY, A. D. (1999) The Hybrid Monte Carlo algorithm on parallel computers. *Parallel Computing* **25** 10-11, 1311 .
- [85] KIBBLE, T. W. B. (1976) Topology of cosmic domains and strings. *J. Phys.* **A9**, 1387.
- [86] KIRKMAN, T. W. and ZACHOS, C. K. (1981) Asymptotic analysis of the monopole structure. *Phys. Rev.* **D24**, 999.
- [87] KISELEV, V. G. (1990) A monopole in the Coleman-Weinberg model. *Phys. Lett.* **B249**, 269.
- [88] KISELEV, V. G. and SELIVANOV, K. G. (1988) Quantum correction to monopole mass. *Phys. Lett.* **B213**, 165.
- [89] KISELEV, V. G. and SHNIR, Y. M. (1998) Forced topological nontrivial field configurations. *Phys. Rev.* **D57**, 5174. [arXiv:hep-th/9801001](#).
- [90] LADAK, S., READ, D. E., PERKINS, G. K., COHEN, L. F. and BRANFORD, W. R. (2010) Direct observation of magnetic monopole defects in an artificial spin-ice system. *Nature Physics* **6**, 359.
- [91] LAMBROU, E. (2011) *Measuring the mass of the topological defect in the 3D Ising model using Monte Carlo simulations*. Master's thesis, Imperial College London.
- [92] LEIMKUHLER, B. and REICH, S. (2005) *Simulating Hamiltonian dynamics* (Cambridge University Press, Cambridge).
- [93] LUSCHER, M. (2010) Computational strategies in lattice QCD [arXiv:1002.4232](#).
- [94] LUSCHER, M. and WOLFF, U. (1990) How to calculate the elastic scattering matrix in two-dimensional quantum field theories by numerical simulation. *Nucl. Phys.* **B339**, 222.
- [95] MANTON, N. S. and SUTCLIFFE, P. (2004) *Topological solitons* (Cambridge University Press, Cambridge).

- [96] METROPOLIS, N., ROSENBLUTH, A. W., ROSENBLUTH, M. N., TELLER, A. H. and TELLER, E. (1953) Equation of state calculations by fast computing machines **21** 6, 1087.
- [97] METROPOLIS, N. and ULAM, S. (1949) The Monte Carlo method. *Journal of the American Statistical Association* **44** 247, 335.
- [98] MICHAEL, C. (1994) Fitting correlated data. *Phys. Rev.* **D49**, 2616.
- [99] MONACO, R., AAROE, M., MYGIND, J., RIVERS, R. J. and KOSHELETS, V. P. (2008) Spontaneous fluxon production in annular josephson tunnel junctions in the presence of a magnetic field. *Phys. Rev. B* **77** 5, 054509.
- [100] MONACO, R., MYGIND, J. and RIVERS, R. J. (2002) Zurek-Kibble domain structures: the dynamics of spontaneous vortex formation in annular Josephson tunnel junctions. *Phys. Rev. Lett.* **89**, 080603.
- [101] MONACO, R., MYGIND, J., RIVERS, R. J. and KOSHELETS, V. P. (2009) Spontaneous fluxoid formation in superconducting loops. *Phys. Rev. B* **80** 18, 180501.
- [102] MONTVAY, I. and MÜNSTER, G. (1997) *Quantum fields on a lattice* (Cambridge University Press, Cambridge).
- [103] MUSSARDO, G. (2007) Neutral bound states in kink-like theories. *Nucl. Phys.* **B779**, 101.
- [104] MUSSARDO, G., RIVA, V. and SOTKOV, G. (2003) Finite-volume form factors in semiclassical approximation. *Nucl. Phys.* **B670**, 464.
- [105] MUSSARDO, G., RIVA, V., SOTKOV, G. and DELFINO, G. (2006) Kink scaling functions in 2D non-integrable quantum field theories. *Nucl. Phys.* **B736**, 259.
- [106] NAKAHARA, M. (1990) *Geometry, topology and physics* (Institute of Physics Press, Bristol).
- [107] NAKAMURA, K. *et al.* (2010) Review of particle physics. *J.Phys.G* **G37**, 075021.

- [108] NEWMAN, M. and BARKEMA, G. (1999) *Monte Carlo methods in statistical physics* (Oxford).
- [109] OHTA, T. and KAWASAKI, K. (1977) Renormalization group approach to the interfacial order parameter profile near the critical point. *Progress of Theoretical Physics* **58** 2, 467.
- [110] PAULI, W. and VILLARS, F. (1949) On the Invariant regularization in relativistic quantum theory. *Rev. Mod. Phys.* **21**, 434.
- [111] PAWELLEK, M. (2009) Quantum mass correction for the twisted kink. *J. Math. Phys.* **42**, 045404. [arXiv:0802.0710](#).
- [112] PESKIN, M. E. and SCHROEDER, D. V. An Introduction to quantum field theory Reading, USA: Addison-Wesley (1995) 842 p.
- [113] PHILIPSEN, O. (2010) Lattice QCD at non-zero temperature and baryon density [arXiv:1009.4089](#).
- [114] PINFOLD, J. L. (1999) Searching for exotic particles at the LHC with dedicated detectors. *Nucl. Phys. Proc. Suppl.* **78**, 52.
- [115] POINCARÉ, H. (1896) Remarques sur une expérience de M. Birkeland. *Compt. Rend. Acad. Sci.* **123**, 530.
- [116] POLCHINSKI, J. (1996) Tasi lectures on D-branes pp. 293–356. [arXiv:hep-th/9611050](#).
- [117] POLYAKOV, A. M. (1974) Particle spectrum in quantum field theory. *JETP Lett.* **20**, 194.
- [118] POLYAKOV, A. M. (1977) Quark Confinement and Topology of Gauge Groups. *Nucl. Phys.* **B120**, 429.
- [119] PÖSCHL, G. and TELLER, E. (1933) Bemerkungen zur quantenmechanik des anharmonischen oszillators. *Zeitschrift für Physik A: Hadrons and Nuclei* **83**, 143.
- [120] PRASAD, M. K. and SOMMERFIELD, C. M. (1975) An Exact Classical Solution for the 't Hooft Monopole and the Julia-Zee Dyon. *Phys. Rev. Lett.* **35**, 760.

- [121] PRESKILL, J. (1984) Magnetic monopoles. *Ann. Rev. Nucl. Part. Sci.* **34**, 461.
- [122] RAJANTIE, A. (2003) Magnetic monopoles from gauge theory phase transitions. *Phys. Rev.* **D68**, 021301. [arXiv:hep-ph/0212130](#).
- [123] RAJANTIE, A. (2006) Mass of a quantum 't Hooft-Polyakov monopole. *JHEP* **01**, 088. [arXiv:hep-lat/0512006](#).
- [124] RAJANTIE, A. and WEIR, D. J. (2009) Quantum kink and its excitations. *JHEP* **04**, 068. [arXiv:0902.0367](#).
- [125] RAJANTIE, A. and WEIR, D. J. (2010) Soliton form factors from lattice simulations. *Phys. Rev.* **D82**, 111502. [arXiv:1006.2410](#).
- [126] RAJANTIE, A. and WEIR, D. J. (2011) Nonperturbative study of the 't Hooft-Polyakov monopole form factors [arXiv:1109.0299](#).
- [127] RAJARAMAN, R. (1987) *Solitons and Instantons* (North-Holland).
- [128] RANDALL, L. and SUNDRUM, R. (1999) A large mass hierarchy from a small extra dimension. *Phys. Rev. Lett.* **83**, 3370. [arXiv:hep-ph/9905221](#).
- [129] REBBI, C. (1980) Phase structure of nonabelian lattice gauge theories. *Phys. Rev.* **D21**, 3350.
- [130] REBBI, C., (ED.) (1984) *Lattice gauge theories and Monte Carlo simulations* (World Scientific, Singapore).
- [131] REBHAN, A., SCHMITT, A. and VAN NIEUWENHUIZEN, P. (2009) One-loop results for kink and domain wall profiles at zero and finite temperature. *Phys. Rev.* **D80**, 045012. [arXiv:0903.5242](#).
- [132] RICHEY, M. (2010) The evolution of Markov Chain Monte Carlo methods. *The American Mathematical Monthly* **117** 5, pp. 383.
- [133] SEGAL, B., BUNCIC, P., SANCHEZ, C. A., BLOMER, J., QUINTAS, D. G., HARUTYUNYAN, A., MATO, P., RANTALA, J., WEIR, D. and YAO, Y. (2010) LHC cloud computing with CernVM. *PoS ACAT2010*, 004.

- [134] SHAO, J. AND TU, D. (1996) *The Jackknife and Bootstrap* (Springer, Berlin).
- [135] SHNIR, Y. M. (2005) *Magnetic monopoles* (Springer, Berlin).
- [136] SIEMENS, X., MANDIC, V. and CREIGHTON, J. (2007) Gravitational wave stochastic background from cosmic (super)strings. *Phys. Rev. Lett.* **98**, 111101.
- [137] SKYRME, T. H. R. (1961) Particle states of a quantized meson field. *Proc. Roy. Soc. Lond.* **A262**, 237.
- [138] SMIRNOV, F. A. (1992) Form-factors in completely integrable models of quantum field theory. *Adv. Ser. Math. Phys.* **14**, 1.
- [139] SMIT, J. (2002) *Introduction to quantum fields on a lattice* (Cambridge University Press, Cambridge).
- [140] SOKAL, A. D. (1989) Monte Carlo methods in statistical mechanics: foundations and new algorithms (lectures given at the Troisieme Cycle de la Physique en Suisse Romande, Lausanne, Switzerland, Jun 15-29, 1989).
- [141] SOKAL, A. D. (1992) Bosonic algorithms. In M. Creutz (ed.), *Quantum fields on the computer*, p. 211 (World Scientific, Singapore).
- [142] SPEIGHT, J. M. (1999) Topological discrete kinks. *Nonlinearity* **12**, 1373. [arXiv:hep-th/9812064](#).
- [143] SUTCLIFFE, P. M. (1997) BPS monopoles. *Int. J. Mod. Phys.* **A12**, 4663. [arXiv:hep-th/9707009](#).
- [144] SWENDSEN, R. H. and WANG, J.-S. (1986) Replica monte carlo simulation of spin glasses. *Phys. Rev. Lett.* **57** 21, 2607.
- [145] 'T HOOFT, G. (1974) Magnetic monopoles in unified gauge theories. *Nucl. Phys.* **B79**, 276.
- [146] TONG, D. (2005) TASI lectures on solitons [arXiv:hep-th/0509216](#).
- [147] TUKEY, J. W. (1958) Bias and confidence in not-quite large samples. *Annals of Mathematical Sciences* **29**, 614.

- [148] VACHASPATI, T. (2004) Reconstruction of field theory from excitation spectra of defects. *Phys. Rev.* **D69**, 043510.
- [149] VACHASPATI, T. and WATKINS, R. (1993) Bound states can stabilize electroweak strings. *Phys. Lett.* **B318**, 163.
- [150] VERSTRAETE, F. and CIRAC, J. I. (2004) Renormalization algorithms for quantum-many body systems in two and higher dimensions [arXiv:cond-mat/0407066](#).
- [151] VIDAL, G. (2007) Entanglement renormalization. *Phys. Rev. Lett.* **99** 22, 220405.
- [152] VILENKIN, A. AND SHELLARD, E. P. S. (2000) *Cosmic strings and other topological defects* (Cambridge University Press, Cambridge).
- [153] WEINZIERL, S. (2000) Introduction to Monte Carlo methods [arXiv:hep-ph/0006269](#).
- [154] WEIR, D. J. (2010) Studying a relativistic field theory at finite chemical potential with the density matrix renormalization group. *Phys. Rev.* **D82**, 025003. [arXiv:1003.0698](#).
- [155] WEIR, D. J. and RIVERS, R. J. (2011) Fluxoid formation: size effects and non-equilibrium universality. *Journal of Physics Conference Series* **286** 1, 012056. [arXiv:1105.2349](#).
- [156] WILSON, K. G. (1974) Confinement of quarks. *Phys. Rev.* **D10**, 2445.
- [157] WU, T. and YANG, C. (1969) In H. Mark and S. Fernbach (eds.), *Properties of Matter Under Unusual Conditions*, p. 349 (Interscience, New York).
- [158] YANG, C.-P. (1963) An approach to the Ising problem. *Proc. Sym. Appl. Math.* **XV**, 351.
- [159] YUROV, V. P. and ZAMOLODCHIKOV, A. B. (1991) Correlation functions of integrable 2-D models of relativistic field theory. Ising model. *Int. J. Mod. Phys.* **A6**, 3419.
- [160] ZUREK, W. H. (1985) Cosmological Experiments in Superfluid Helium? *Nature* **317**, 505.

- [161] ZUREK, W. H. (1996) Cosmological Experiments in Condensed Matter Systems. *Phys. Rept.* **276**, 177. [arXiv:cond-mat/9607135](#).